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"COMPUTER MODELS OF SOLIDS-FLUID CHEMICAL REACTORS
AND
CORRELATION OF MULTIVARIATE DATA"

by

P.K. Leung

A THESIS

SUBMITTED TO THE FACULTY OF GRADUATE STUDIES
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The undersigned certify that they have read, and recommend to the Faculty of Graduate Studies for acceptance, a thesis entitled "Computer Models of Solids-Fluid Chemical Reactors and Correlation of Multivariate Data" submitted by P.K. Leung, B.Sc. in partial fulfilment of the requirements for the degree of Doctor of Philosophy in Chemical Engineering.

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ABSTRACT

In the first part of this thesis solid-fluid chemical reactors, with reaction if any only in the fluid phase, are simulated mathematically with due consideration of the temperature gradients in the solid particles. A heat diffusion equation describes the temperature change with time in the solid spheres, a separate equation describes the gas temperature along the reactor. They are coupled together by the boundary condition on the surface of the solids. If reaction is present additional equations for component balances along the reactor are also included.

For a moving bed reactor, assuming a uniform velocity of the bed, the system can be readily expressed by a set of simultaneous ordinary differential equations, having z the length along the reactor as the sole independent variable, the dependent variables being composition, temperature and pressure of the fluid and a series of temperatures along the radius of the solid particles. It is then solved firstly by an analog computer for no chemical reaction, and numerically by the Runge-Kutta-Gill method in a digital computer for both cases with and without chemical reactions.

However, in the fixed bed regenerative reactor the time variables for both the solid and gas are different. The above approach is not applicable. A mathematical model is proposed in which the surface temperature in a differential

volume of the reactor is assumed to change linearly with time, so that the gas phase in passing through this reactor volume sees the mean surface temperature of the solid. Thus, the equations describing the gas phase and the solid phase are effectively decoupled. With an assumed final surface temperature for a given time, an analytical solution can be obtained for the solid phase; the gas phase is described by a set of ordinary differential equations which, with the mean surface temperature as a parameter, can be readily solved numerically. The correct final surface temperature is established through trial-and-error using an energy balance on the two phases.

The above proposed methods had been tested numerically against known solutions for simple cases or against established methods for more general cases and found to be accurate and feasible.

The latter part of the thesis involves the study of the correlation of multivariate data. A least squares analysis with self-generating orthogonal polynomials as approximating functions was used for curve fitting. It was found to be most convenient to use and gave good accuracy for high order approximations. This approach was developed to surface fitting, with two independent variables. The results obtained indicate the reliability and the accuracy of this method.

If the approximating functions are of some specified form the polynomial approach will no longer be applicable.

If the Chebyshev criterion of fit can be used, then the analysis becomes a linear programming problem with the maximum absolute deviation to be minimized as the objective function. The problem can be solved more readily through its dual, using the Simplex method. A program for the Simplex method has been developed for the dual problem in search for the optimal base. Thus, a corresponding optimal in the primal can be obtained, which is a set of equations equal to the number of coefficients plus the minimal maximum deviation. This may be solved by any conventional method.

It was applied to curve fitting and the evaluation of Benedict-Webb-Rubin equation of state. The results of the approximation illustrate the accuracy of the method.

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PART ONE

COMPUTER MODELS OF SOLIDS-FLUID CHEMICAL REACTORS

- REACTIONS IN FLUID PHASE ONLY

I. INTRODUCTION

Solids-gas contacting operations are among the most important and widely encountered in the chemical metallurgical and petroleum industries. A detailed description of this operation is given by Vener and Robinson(1). From the point of view of chemical engineering, solids-gas contacting should be considered as a broad unit operation, in which moving-bed, fixed-bed and fluidized-bed techniques may be considered as some typical examples.

In the processes of adsorption, drying or solvent removal, thermal decomposition of solids, thermal cracking and pebble-bed heat exchangers, the temperature or concentration gradients in the solids are of prime concern in the design of the reactors. It is the purpose of this thesis to study the temperature or concentration profiles along the reactors at various times of the operation with due consideration of the temperature or concentration gradients in the solids. However, in the fluidized bed the solid diameters are so small that the temperature gradients in the solids can probably be neglected. Thus, only moving beds and fixed beds will be studied in the following sections.

A moving bed can be defined as a body of solid particles moving downward by gravity in a reactor, through which gas may flow parallel or countercurrent to the solids. Due to its ability to handle a wide variety of solids,

elimination of dust entrainment problems, reasonable pressure drops, simple provisions for establishing desirable temperature gradients along the reactor to permit optimum conversions, uniformity in residence time of solids, suitable temperature control by various heat transfer techniques and many other advantages, the moving bed process is considered to have one of the best growth potentials in the solids-gas contacting field(2).

The process of bringing gases into contact with fixed solids is even more common. A fixed bed may be defined as a body of solid particles packed in a reactor through which gases may pass upward or downward. As compared to the moving bed, the main advantage of fixed bed processes is the lack of necessity of equipment for circulating the solids. However, owing to the relatively poor heat transfer characteristics, excessive temperature gradients often exist within the bed.

The problems to be considered involve the calculation of the behavior of a flowing gas stream and a moving bed or fixed bed of solids, where chemical reaction, if any occurs only in the gas phase. The analysis is predicated upon the following assumptions: no radial temperature or concentration gradients in the gas phase, i.e. one-dimensional reactor; no axial dispersion of either energy or mass except by bulk flow; the solids are homogeneous uniform-sized spheres; the reactors are adiabatic; and the particles are large enough so

that internal temperature or concentration gradients are significant but small enough so that the fluid environment can be considered as uniform, thus ensuring radial symmetry.

II. STUDIES OF FINITE DIFFERENCE TECHNIQUES IN HEAT TRANSFER BETWEEN SOLIDS AND GAS

Before attempting to solve the design problem, it is appropriate to consider the techniques which are presently used in simple systems.

Consider a sphere of homogeneous and isotropic solid, having initial temperature T_0 . It is submerged at time zero into a well-stirred fluid of constant temperature, T_g . The temperature distribution in the sphere at any time is required.

Mathematically

$$\frac{\partial T}{\partial t} = K \left(\frac{\partial^2 T}{\partial r^2} + \frac{2}{r} \frac{\partial T}{\partial r} \right) \quad (\text{II.1})$$

with boundary conditions of

$$\frac{\partial T}{\partial r} = 0 \quad r = 0$$

$$\frac{\partial T}{\partial r} = \frac{h_f}{k_s} (T_g - T_s) \quad r = R \quad (\text{II.2})$$

$$T_s = T \quad r = R$$

and initial condition

$$T = T_0 \quad t = 0 \quad \text{for } 0 \leq r < R \quad (\text{II.3})$$

This system is to be solved by three different methods, namely, 1) analytical, 2) implicit and 3) explicit method.

1) Analytical Method:

By separation of variables, equation (II.1) can be readily solved to give

$$T = T_g + \sum_{n=1}^{\infty} \sqrt{\frac{2}{a_n \pi}} \left\{ \exp(-K a_n^2 t) \right\} \frac{A_n \sin a_n r}{r} \quad (\text{II.4})$$

where a_n are the roots of the transcendental equation

$$\tan(a_n R) = \frac{(a_n R) k_s}{k_s - R h_f} \quad (\text{II.5})$$

The constants A_n are the coefficients of the orthogonal functions in approximating the initial temperature distribution and are given as

$$\begin{aligned} A_n &= \frac{\int_0^R r^2 \sqrt{\frac{2}{a_n \pi}} \left\{ (\sin a_n r)/r \right\} (T_o - T_g) dr}{\int_0^R r^2 \left(\frac{2}{a_n \pi} \right) (\sin a_n r)^2 / r^2 dr} \\ &= \sqrt{\frac{2\pi}{a_n}} (T_o - T_g) \frac{\sin a_n R - a_n R \cos a_n R}{a_n R - 1/2 \sin 2a_n R} \quad (\text{II.6}) \end{aligned}$$

2) Implicit (Crank-Nicholson) Method:

According to the implicit expression proposed by Crank-Nicholson(3), the finite difference representation of equation (II.1) according to the network given in Figure 1a,

is

$$\begin{aligned}
 & \left[(6W + 1)T_1 - 6WT_2 \right]_{k+1} = \left[(1 - 6W)T_1 + 6WT_2 \right]_k \\
 & \left[WT_1 + (1 + 2W/3)T_2 - (5W/3)T_3 \right]_{k+1} = \left[-WT_1 + (1 - 2W/3)T_2 + (5W/3)T_3 \right]_k \\
 & \left[-Wj'/3 T_{j-2} - W(1 - 2j')T_{j-1} + (1 - W(j' - 2))T_j \right. \\
 & \quad \left. - W(1 + 2j'/3)T_{j+1} \right]_{k+1} \\
 & = \left[Wj'/3 T_{j-2} + W(1 - 2j')T_{j-1} + (1 + W(j-2))T_j \right. \\
 & \quad \left. + W(1 + 2j'/3)T_{j+1} \right]_k
 \end{aligned}$$

$$\text{for } j = 3, 4, 5, \dots, M-1 \quad (\text{II.7})$$

$$\begin{aligned}
 & \left[(-WM'/3 - 2C)T_{M-2} - (W(1 - 2M') - 9C) T_{M-1} \right. \\
 & \quad \left. + (1 - W(M' - 2) - 18C)T_M \right]_{k+1} \\
 & = \left[(WM'/3 + 2C)T_{M-2} + (W(1 - 2M') - 9C) T_{M-1} \right. \\
 & \quad \left. + (1 + W(M' - 2) + 18C) T_M \right]_k + 2BCT_g
 \end{aligned}$$

where $T_{M+1} = (2T_{M-2} - 9T_{M-1} + 18T_M + BT_g)/(11 + B)$ (II.8)

and

$$W = \frac{\Delta t \cdot K}{2 \cdot \Delta r^2}, \quad B = \frac{12 \Delta r h_f}{k_S}, \quad j = \frac{1}{(j - 1)}$$

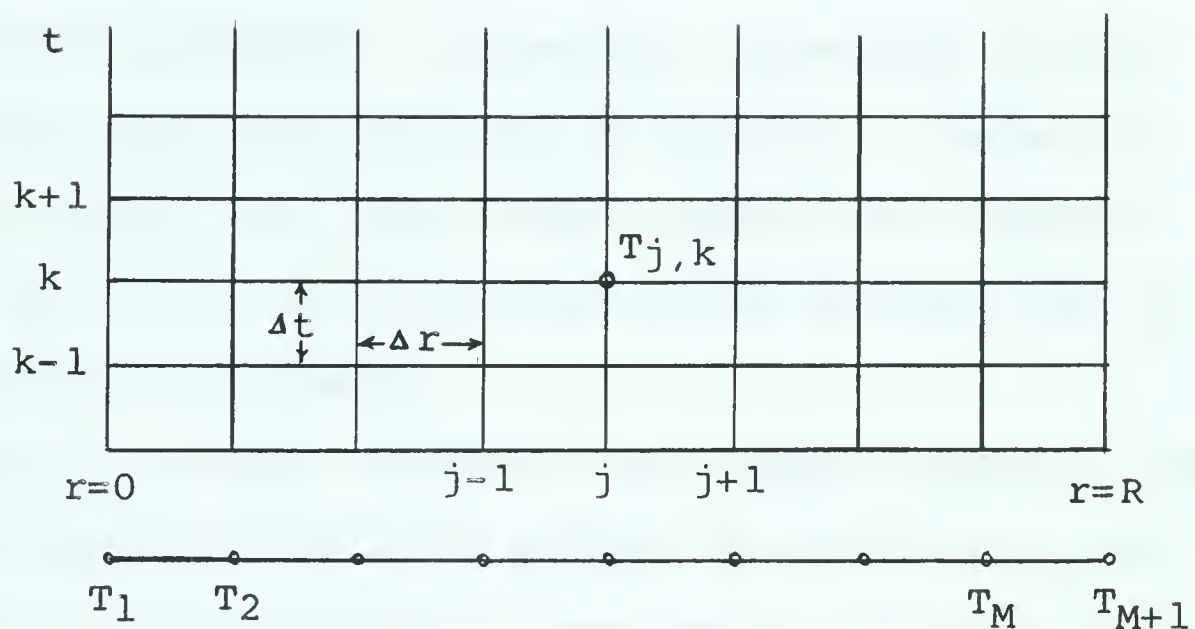
$$M' = 1/(M-1), \quad C = W(1 + 2M'/3)/(11 + B)$$

Expression (II.7) is the final computational system. Other

Figure 1

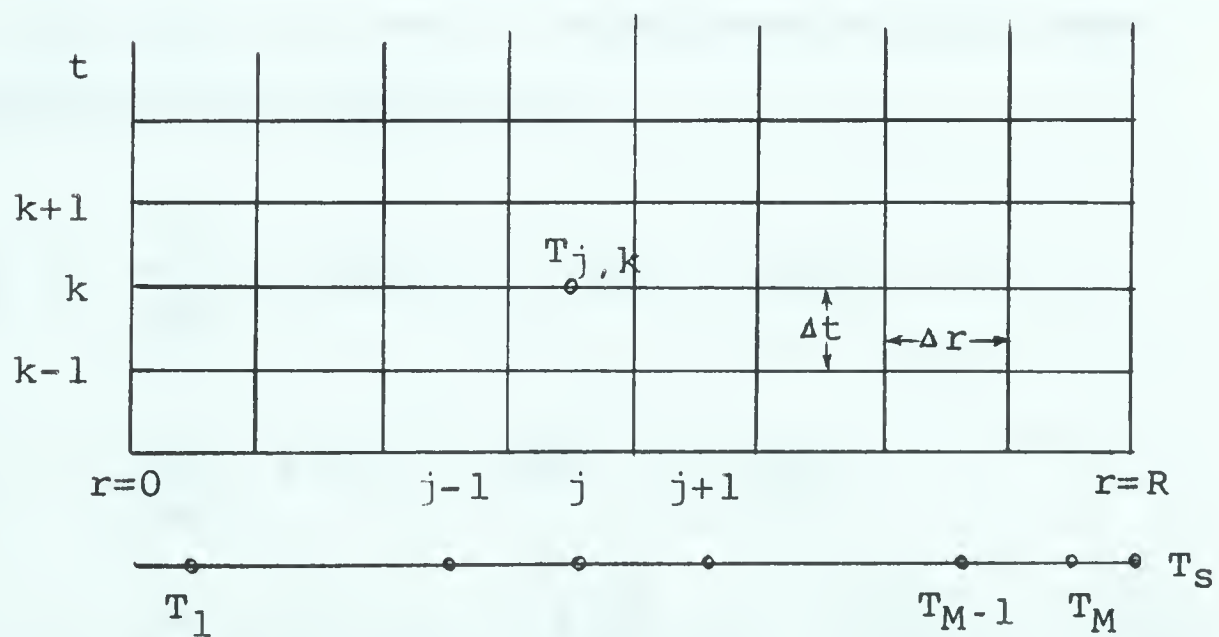
Network for Heat Conduction Equation.

(a)



$$T_{j,k} = T(j\Delta r, k\Delta t)$$

(b)



$$T_{j,k} = T((j-\frac{1}{2})\Delta r, k\Delta t)$$

forms of implicit expressions are possible and are discussed in detail by Lapidus(4).

3) Explicit (Runge-Kutta-Gill) Method:

The original form of this numerical integration of ordinary differential equations was due to Runge(5), but was later modified by Kutta(6). A complete derivation of the method is very complicated and can be found in a paper by Ince(7). The method has been further refined for digital computation by Gill(8) so as to give better accuracy and to minimize storage requirements.

Here R is again divided into M equal sections, with discrete functional values of T assumed to be in the middle of each section, representing the mean value of the spherical shell as sketched in Figure 1b. Now third order correct expressions are used for $\partial T / \partial r$ and $\partial^2 T / \partial r^2$ as derived in Appendix A. Thus, equation (II.1) and its associated boundary conditions give rise to a set of simultaneous first order ordinary differential equations as

$$DT_1 = \frac{K}{8\Delta r^2} (-26T_1 + 27T_2 - T_3)$$

$$DT_2 = \frac{K}{9\Delta r^2} (-T_1 - 12T_2 + 13T_3)$$

$$DT_j = \frac{K}{\Delta r^2} \left(\frac{2}{6j-3} T_{j-2} + \frac{2j-5}{2j-1} T_{j-1} - \frac{4j-4}{2j-1} T_j + \frac{6j+1}{6j-3} T_{j+1} \right)$$

$$j = 3, 4, \dots, M-1$$

$$DT_M = \delta \left\{ (9\gamma - 12M + 18)T_{M-2} - (50\gamma - 120M + 140)T_{M-1} \right. \\ \left. + (225\gamma - 300M + 90)T_M + \beta \cdot \gamma \cdot T_g \right\} \quad (\text{II.9})$$

where

$$D = d/dt$$

$$\beta = 60\Delta r h_f / k_s$$

$$\gamma = (192M + 32) / (184 + \beta)$$

$$\delta = K / (\Delta r^2 \cdot 30(2M-1))$$

However at $r = R$

$$\frac{\partial T_s}{\partial r} = \frac{h_f}{k_s} (T_g - T_s)$$

$$= (184T_s - 225T_M + 50T_{M-1} - 9T_{M-2}) / (60\Delta r)$$

$$\therefore T_s = (\beta T_g + 225T_M - 50T_{M-1} + 9T_{M-2}) / (184 + \beta) \quad (\text{II.10})$$

System (II.9) is then integrated numerically by the Runge-Kutta-Gill method which is described in Appendix B. It can be seen that the computational program for the explicit formula (II.9) is quite simple and direct in comparison with that of the implicit formula (II.7). However, there are some severe computational restrictions involved in the use of the formula. The stability requirement may demand such small time increments that computing times become excessive. An analysis of the stability is presented in Appendix C.

II.1 Numerical Example

For numerical evaluation, the following specific values are used:

$$T_o = 0$$

$$R = 0.1 \text{ (ft)}$$

$$h_f = 50 \text{ BTU/}(\text{hr})(\text{ft}^2)$$

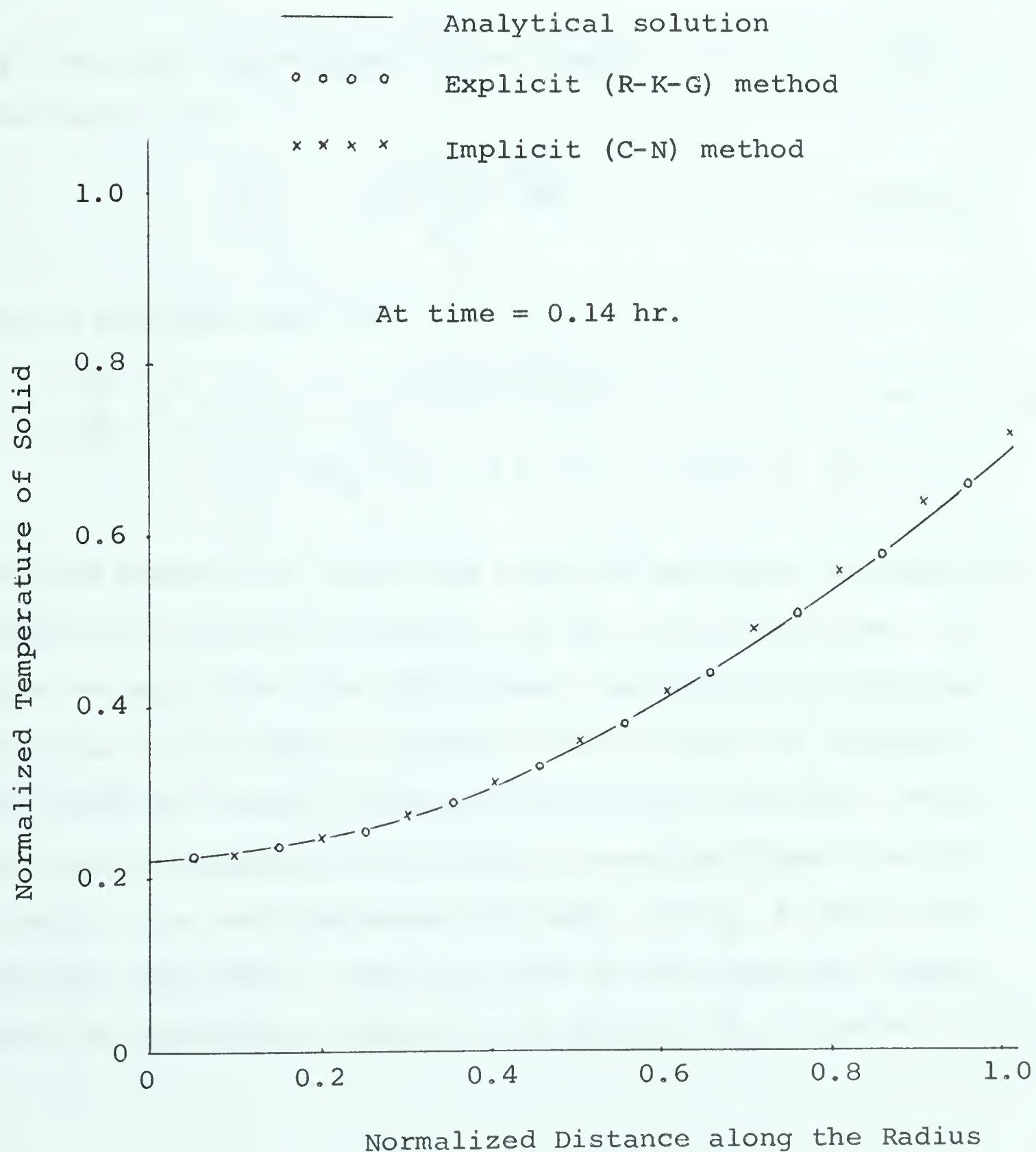
$$k_s = 2.0 \text{ BTU/}(\text{hr})(\text{ft}^2)(^\circ\text{F}/\text{ft})$$

$$T_g = 1.0$$

$$\Delta r = 0.01 \text{ (ft)}$$

$$K = 0.01 \text{ (ft}^2\text{)}/(\text{hr})$$

The results from the above three methods are plotted in Graph No. 1, which shows that the Runge-Kutta method gives slightly better accuracy than that of the implicit Crank-Nicholson method. This difference in the results is expected as the finite difference representation of $\partial T / \partial t$ is fourth order correct for the Runge-Kutta method, but only second order correct for the implicit method. However, the implicit method cannot be conveniently used if any of the differential equations are non-linear.

Graph No. 1Comparison of Results by Various Finite Difference
Methods in Heat Conduction.

III. MOVING BED CHEMICAL REACTOR DESIGN

For a differential section of the reactor, the energy balance in the gas phase is

$$\frac{dT_g}{dz} = \frac{-4(h_w/D_R)(T_g - T_w) - h_f k_s(T_g - T_s) + R(x, P, T_g)\Delta H_T}{G_m C_{p_m}} \quad (\text{III.1})$$

The fractional conversion of the limiting reactant in the flow reactor is

$$\frac{dx}{dz} = \frac{R(x, P, T_g)}{G_m^O} \quad (\text{III.2})$$

and the pressure drop is

$$\frac{dP}{dz} = \frac{1.635 G^2 (1 - \epsilon)}{\left\{ (1.77 D_p \frac{G}{\mu} (1 - \epsilon))^{0.05} - 0.81 \right\} g_c D_p \epsilon^3 \rho_g} \quad (\text{III.3})$$

which is proposed by Ergun and modified by Glaser and Thodos(9) to take into account the motion of the solid particles. If there are more than one independent reaction then additional equations of the form of equation (III.2) must be included. Both axial and radial diffusions have been neglected. These then are the equations describing a one-dimensional reaction in which z is the independent variable and T_g , X and P the dependent variables. The only term in the equations, which cannot be immediately expressed in terms of T_g , X and P , is T_s ,

the surface temperature of the moving bed of solids. To evaluate it, an energy balance must be written about the solid-gas interface.

Therefore, attention must now be focussed on the solid phase, where the thermal behavior of a homogeneous solid sphere is given by

$$\frac{\partial T}{\partial t} = K \left(\frac{\partial^2 T}{\partial r^2} + \frac{2}{r} \frac{\partial T}{\partial r} \right) \quad (\text{III.4})$$

where K , the thermal diffusivity ($k_s/\rho_s c_s$) is assumed to be independent of r and T .

In the problem under study, since the solids are moving through the reactor at a constant rate, t and z are related linearly and equation (III.4) may be written as

$$\frac{\partial T}{\partial z} = B \left(\frac{\partial^2 T}{\partial r^2} + \frac{2}{r} \frac{\partial T}{\partial r} \right) \quad (\text{III.5})$$

where

$$B = \frac{K \rho_s (1 - \epsilon)}{G_s}$$

The boundary conditions are

$$\begin{aligned} \frac{\partial T}{\partial r} &= 0 & r &= 0 \\ \frac{\partial T}{\partial r} &= \frac{h_f}{k_s} (T_g - T_s) & r &= R \end{aligned} \quad (\text{III.6})$$

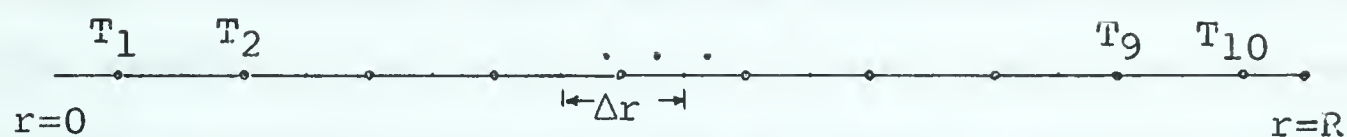
and initial conditions are

$$\begin{aligned} T &= T_0 \\ T_g &= T_g^0 \\ X &= X_0 \\ P &= P_0 \end{aligned} \quad \text{at } z = 0$$

The complexity of the solution depends upon the relationship that exists between T_s and other variables. Furthermore, equations (III.1) to (III.3) are inherently non-linear. In essence, the problem involves the solution of a second order, parabolic partial differential equation describing the solid, a set of first order ordinary differential equations describing the gas, coupled by a heat transfer rate equation (III.6) at the gas-solid interface.

The proposed solution uses numerical finite difference methods, outlined partly in section II. The first step is to convert the partial differential equation (III.5) into a set of ordinary equations by replacing $\partial T / \partial r$ and $\partial^2 T / \partial r^2$ at various discrete values of r , with their appropriate finite-difference expressions from Appendix A. As recommended in section II, the network in Figure 1b is used and the various equations are shown in Table 1.

The system of differential equations to be solved comprise equations (III.1), (III.2), (III.3) and the set (III.7). The numerical solution of these equations, much too formidable

TABLE 1Differential Equations for TemperatureDistribution in Spheres

$$\frac{dT_1}{dz} = \frac{B'}{8} (-26T_1 + 27T_2 - T_3)$$

$$\frac{dT_2}{dz} = \frac{B'}{9} (-T_1 + 12T_2 + 13T_3) \quad (\text{III.7})$$

$$\begin{aligned} \frac{dT_j}{dz} = B' & \left(\frac{2}{6j-3} T_{j-2} + \frac{2j-5}{2j-1} T_{j-1} \right. \\ & \left. - \frac{4(j-1)}{2j-1} T_j + \frac{6j+1}{6j-3} T_{j+1} \right) \end{aligned}$$

$$\begin{aligned} \frac{dT_{10}}{dz} = \delta & ((9\gamma - 102) T_8 - (50\gamma - 1060) T_9 \\ & + (225\gamma - 2910) T_{10} + \gamma\beta T_9) \end{aligned}$$

where

$$B' = B/\Delta r^2$$

$$\beta = \frac{60 \Delta r h_f}{k_s}$$

$$\gamma = 1888/(184 + \beta)$$

$$\delta = B'/570$$

to attempt by hand calculations, is now possible and practicable with digital or analog computers.

The problem is treated as an initial value problem, which would be the case for cocurrent flow. All the variables are known at some one value of the independent variable, namely at the reactor inlet, i.e. $z = 0$. For countercurrent reactors the initial values of X , P and T_g would have to be assumed and the solution is obtained by trial-and-error. The Runge-Kutta-Gill method, outlined in Appendix B, is used for the numerical integration.

Before numerical examples are presented, an alternative approach will be discussed. One of the most powerful tools for solving sets of simultaneous ordinary differential equations is the analog computer, which by its inherently parallel operation avoids the problem of stability encountered in finite-difference methods. The linear differential equations can be simulated on an analog computer with a high degree of accuracy and require comparatively little equipment - about four amplifiers per equation. The non-linear equations require the use of special function generators which have a lower degree of accuracy and require a great many more electronic components. In fact, it is fair to say that the difficulty of generating non-linear terms is the biggest physical problem in using analog computers. There is, however, no inherent theoretical limitation to the solution of such sets of differential equations by analog computers.

As a check on the accuracy of the methods proposed, two numerical example problems have been solved.

III.1 Example Problem No. 1

This example problem on moving bed heat exchanger was presented in Amundson's paper(10):

Limestone is calcined in a continuous countercurrent vertical lime kiln. The calcium carbonate is fed in at the top in 2" pieces at a superficial mass velocity of 230 pounds per square foot per hour. Flue gas and carbon dioxide from the calcination rise through the bed at a superficial mass velocity of 2500 pounds per square foot per hour. If the limestone enters at 100°F and the gas leaves at 200°F, what is the temperature distribution in the kiln as a function of distance from the top, assuming no chemical reaction?

Physical data are

specific heat of gas	= 0.25 BTU/(lb)(°F)
specific heat of calcium carbonate	= 0.28 BTU/(lb)(°F)
density of calcium carbonate	= 162 lb/(ft ³)
heat transfer coefficient	= 78 BTU/(hr)(ft ²)(°F)
thermal conductivity of calcium carbonate	= 1.3 BTU/(hr)(ft)(°F)
fractional void space	= 0.50

Since there is no chemical reaction present and the kiln is assumed to be adiabatic, without consideration of the pressure drop, the gas phase is, therefore, described as

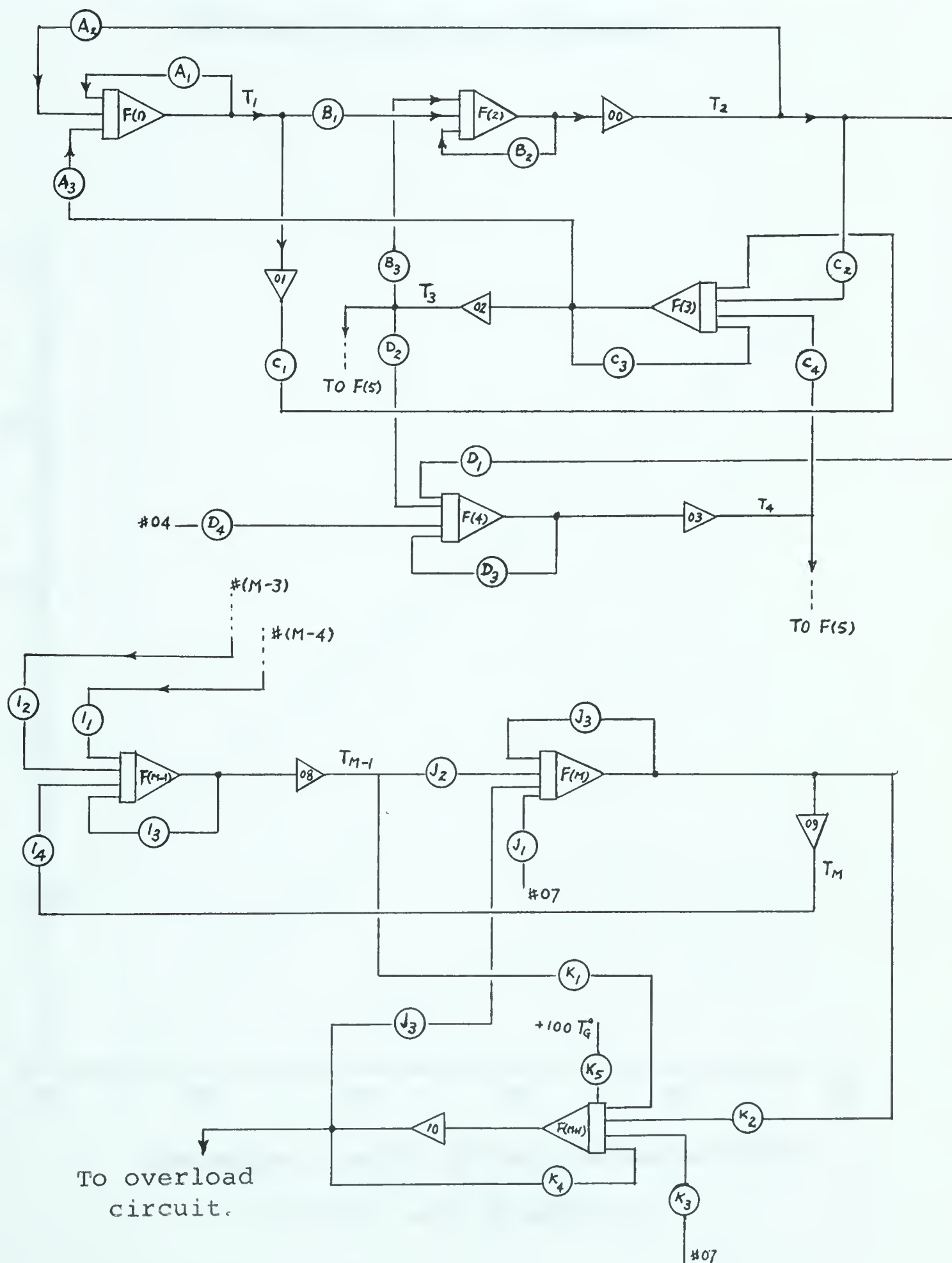
$$\begin{aligned}
 \frac{dT_g}{dz} &= \frac{h_f A_s (T_g - T_s)}{G C_f} \\
 &= \frac{3(1 - \epsilon) h_f (T_g - T_s)}{G C_f R} \quad (\text{III.8})
 \end{aligned}$$

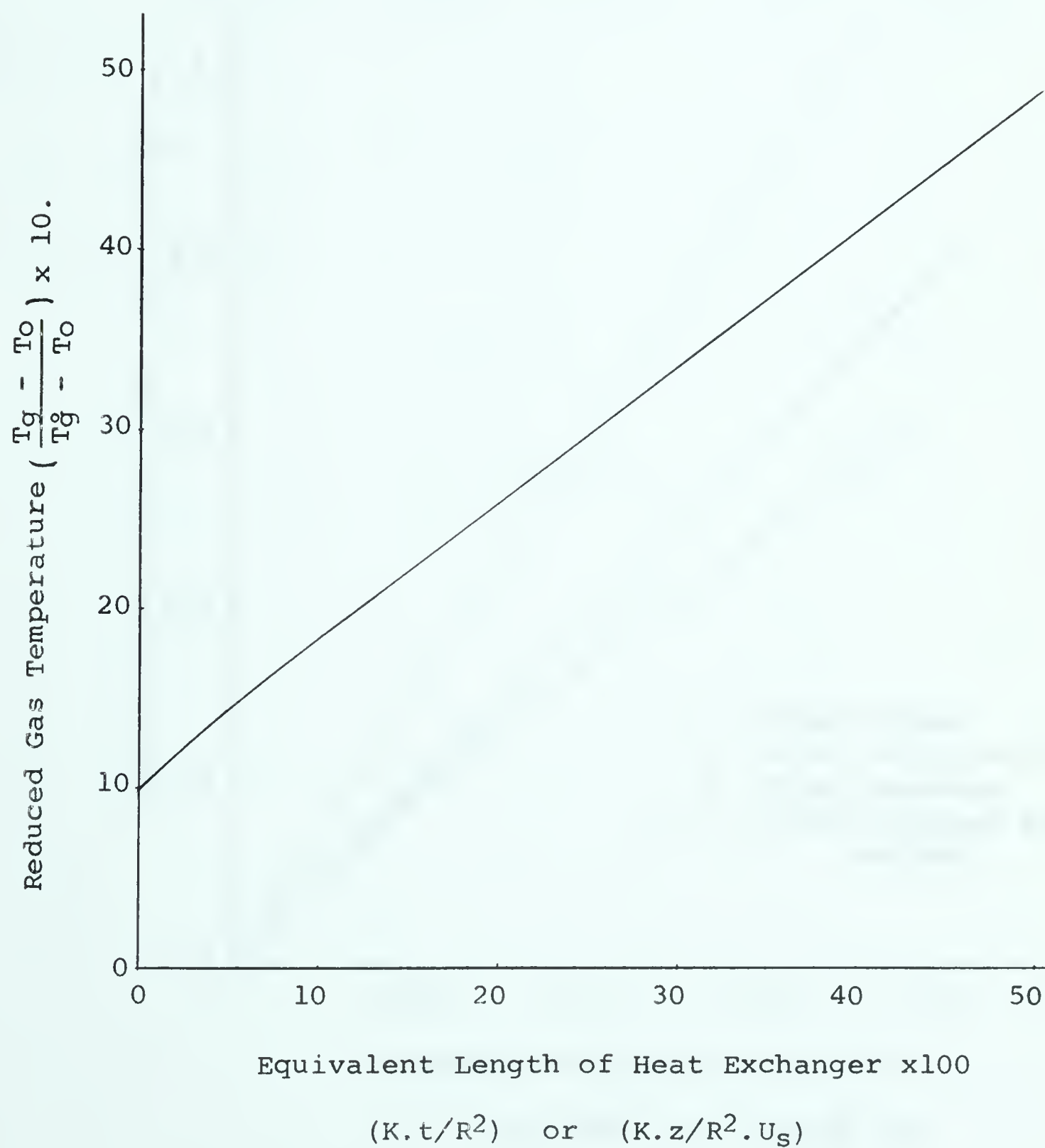
Together with equation (III.7), they form a set of simultaneous linear first order ordinary differential equations. A Pace 231R analog computer was used to obtain solution. The circuit diagram for this case is shown in Figure 2 and the result generated by the X-Y plotter is given in Graph No. 2. The numerical solution, obtained by the Runge-Kutta-Gill method, was performed on an I.B.M. 1620 digital computer. The program, written in Fortran IV, is listed in Appendix F.

This problem has been solved by Furnas(11) analytically in neglecting conduction in the solid, by Lovell and Karnofsky(12) using a modified Schmidt method, and by Amundson(10) using successive Laplace transformations to give the exact solution. Results from the above methods are plotted in Graph No. 3 for comparison. It is obvious that the results of the proposed method very nearly coincide with those by Amundson. As a better comparison the results are tabulated in Table 2. This confirms the accuracy, both of the finite difference expressions and of the integrative technique used.

Figure 2

Analog Computer Circuit Diagram for
Moving Bed Heat Exchanger.



Graph No. 2Temperature Profile for Moving Bed HeatExchanger from Analog Computer.

Graph No. 3

Temperature Profiles along the Moving-bed Reactor
in countercurrent system

with $(G_s.C_s/G_a.C_f) = 1.0$
 $(k_s/h_f.R) = 0.2$

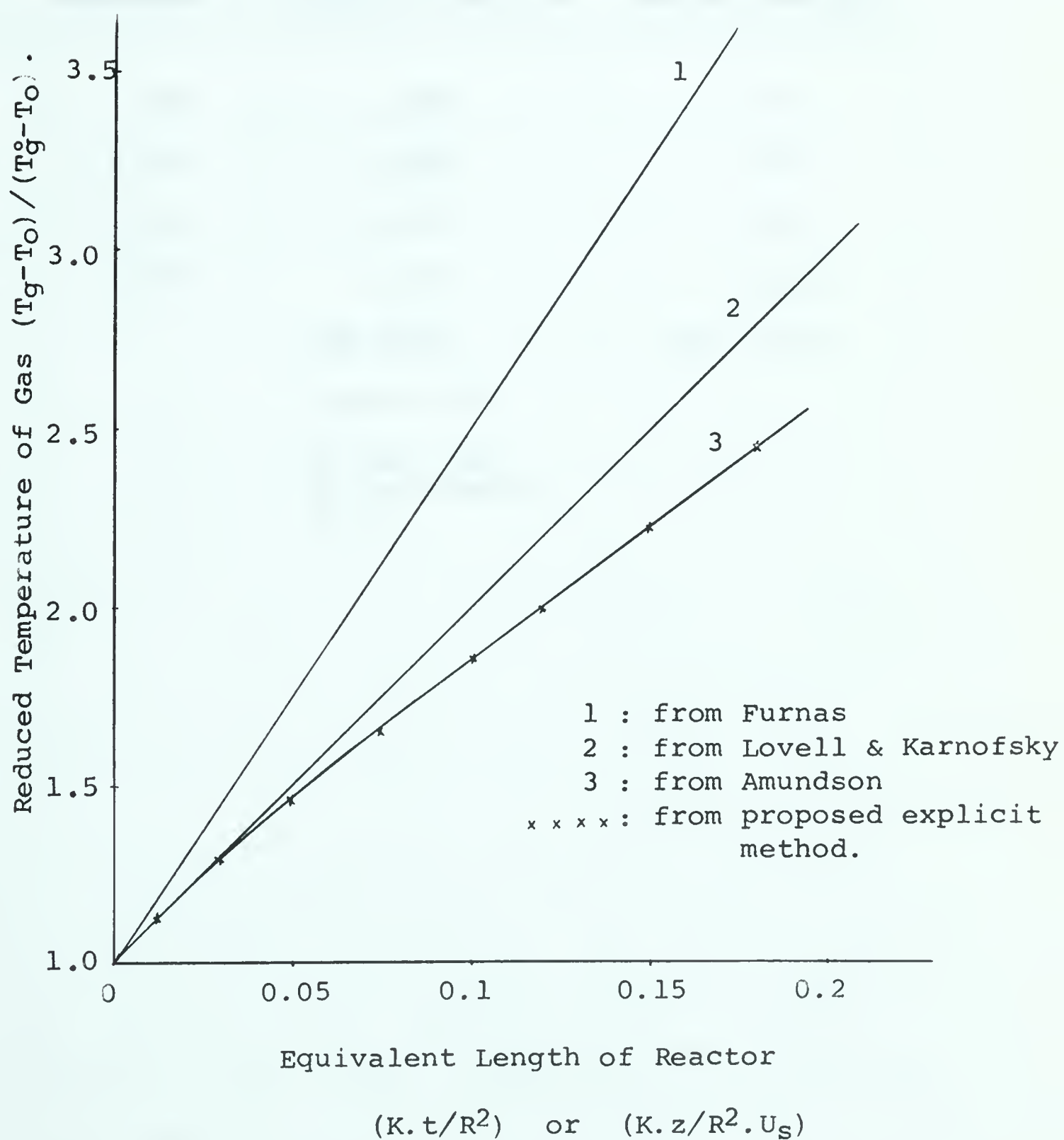


TABLE 2Comparison of Solutions in Moving-BedHeat Exchanger Example

Equivalent Length of Exchanger (Kz/R^2u_s)	Reduced Temperature ($\frac{T_g - T_o}{T_{go} - T_o}$)		
	Analytical Solution by Amundson	Explicit Solution by Digital Computer	Explicit Solution by Analog Computer
0.05	1.46	1.458	1.47
0.10	1.85	1.848	1.85
0.15	2.23	2.227	2.22
0.1854	2.50	2.494	2.500
		IBM 7040	Pace 231R
		Fortran IV	
		20 sec. for 63 increments in z	

III.2 Example Problem No. 2

This problem, taken from Walas' "Reaction Kinetics for Chemical Engineers"(13) is given as follows:

Butane is cracked in a moving bed pebble heater, according to the following reaction,



with

$$\Delta H_{60^\circ\text{F}} = 98,600 \text{ BTU/lb-mole converted}$$

$$\Delta H_{1200^\circ\text{F}} = 99,100 \text{ BTU/lb-mole converted}$$

The reaction is first-order with

$$\log k = -22,100/T_g + 12.45$$

where T_g is in $^\circ\text{R}$ and k in sec^{-1} .

The pebbles are alumina spheres 5/16 inch in diameter and have a heat capacity of 25 BTU/(cu.ft.)($^\circ\text{F}$), a surface area of 126 sq.ft./(cu.ft.), and a void fraction of 0.45. After preheated uniformly to 2000 $^\circ\text{F}$ the pebbles are allowed to flow downward through the reactor in parallel to butane, which enters at 500 $^\circ\text{F}$ and 20 psig. The butane flow rate is 42.6 lb-moles/(hr)(sq.ft.) and the pebble rate is 682 cu.ft. per (hr)(sq.ft.). The heat transfer coefficient from the gas to the pebbles is 97.6 BTU/(hr)(sq.ft.)($^\circ\text{F}$). It is desired to calculate the length of reactor required to obtain various fraction conversion of the butane. Property values of the gas are given in the text.

For the first-order reaction (III.9) if the gas is assumed to behave ideally, then the rate of reaction is given by

$$R(x, p, T_g) = kC_a$$

$$= \frac{k \cdot P \cdot (1 - X)}{R' \cdot T_g \cdot (1 + 2X)} \quad \left(\frac{\text{lb-mole}}{\text{hr ft}^3} \right) \quad (\text{III.10})$$

where C_a is the concentration of n-butane
 X is the fractional conversion of n-butane in terms of total feed
 P is the total pressure

$$\frac{dx}{dz} = \frac{\{ P \cdot (1 - X) \cdot \exp(12.45 - 22100/T_g) \}}{G_m^0 \cdot R' \cdot T_g \cdot (1 + 2X)} \quad (\text{III.11})$$

If T_b is the reference temperature then equation (III.1) can be written as

$$\frac{dT_g}{dz} = \frac{\frac{h_f A_s}{G_m^0} (T_s - T_g) - \left\{ (-Cp_1 + 2Cp_2 + Cp_3) (T_g - T_b) + \Delta H_{T_b} \right\} \frac{dx}{dz}}{((1 - X) \cdot Cp_1 + 2XCp_2 + XCp_3)} \quad (\text{III.12})$$

where Cp_1 , Cp_2 , Cp_3 are the molar specific heats of n-butane, ethylene and hydrogen respectively.

The density at any point in the reactor for ideal gas behavior is given as

$$\begin{aligned}
 p_f &= \frac{58}{(1 + 2X)(379)\left(\frac{T_g}{520}\right)\left(\frac{14.7}{P}\right)} \\
 &= \frac{5.4P}{(1 + 2X) \cdot T_g} \quad (\text{III.13})
 \end{aligned}$$

so that with mean values for μ equation (III.3) can be simplified into

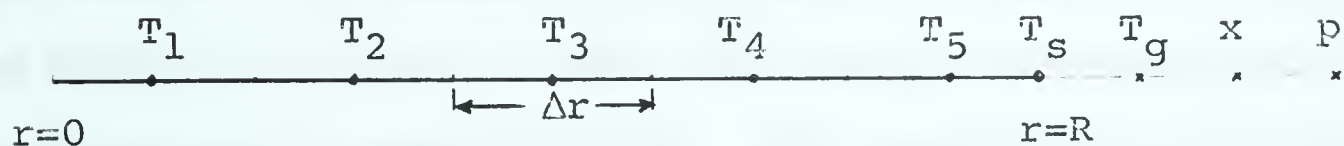
$$\frac{dp}{dz} = 0.01 \times \frac{(1 + 2X) T_g}{P} \quad (\text{III.14})$$

As the solid radius is not too large it is sufficient to divide it into 5 equal sections so that equation (III.5) is expressed into a set of but 5 equations, listed in Table 3.

The complete set of equations for computation includes (III.15) for the solid and (III.11), (III.12), (III.14) for the gas. It can be seen that the equations describing the gas phase are non-linear, so that analytical solution is impossible. However, in the solution by Walas, the internal temperature of the pebbles is considered to be uniform and, therefore, the thermal conductivity of the pebbles does not enter into the calculations. Thus, with finite increments along the reactor length, a solution by trial-and-error for the gas temperature at the end of each increment can be obtained. In the present proposed method, the set of equations for the system was solved numerically by

TABLE 3

The Computational System for Solid in the
Moving Bed Reactor



$$\frac{dT_1}{dz} = \frac{B'}{8} (-26T_1 + 27T_2 - T_3)$$

$$\frac{dT_2}{dz} = \frac{B'}{9} (-T_1 - 12T_2 + 13T_3)$$

$$\frac{dT_3}{dz} = \frac{B'}{15} (2T_1 + 3T_2 - 24T_3 + 19T_4) \quad (\text{III.15})$$

$$\frac{dT_4}{dz} = \frac{B'}{21} (2T_2 + 9T_3 - 36T_4 + 25T_5)$$

$$\begin{aligned} \frac{dT_5}{dz} = & \delta ((9\gamma - 42)T_3 - (50\gamma - 460)T_4 \\ & + (225\gamma - 1410)T_5 + \gamma\beta T_g) \end{aligned}$$

where $B' = B/\Delta r^2$

$$\beta = (60 \Delta r h_f)/k_s$$

$$\gamma = 983/(184 + \beta)$$

$$\delta = B'/(270)$$

the Runge-Kutta-Gill method, using a pebble thermal conductivity of $1.8 \text{ BTU}/(\text{hr} \cdot \text{ft} \cdot ^\circ\text{F})$.

The results of the different methods are illustrated in Graphs No. 4a and 4b for the fractional conversion and the gas temperature profiles respectively. The differences are considerable. By comparing the results tabulated in Table 4a, from Walas, with those in Table 4b from proposed explicit method, the difference becomes obvious. The temperature difference between gas and solid is as high as 300°F for the greater part of the reactor in the former, while in the latter, it is less than 100°F . In fact the temperature gradients in the solid can be found to be at least 15°F for half of the reactor length, which is certainly not negligible.

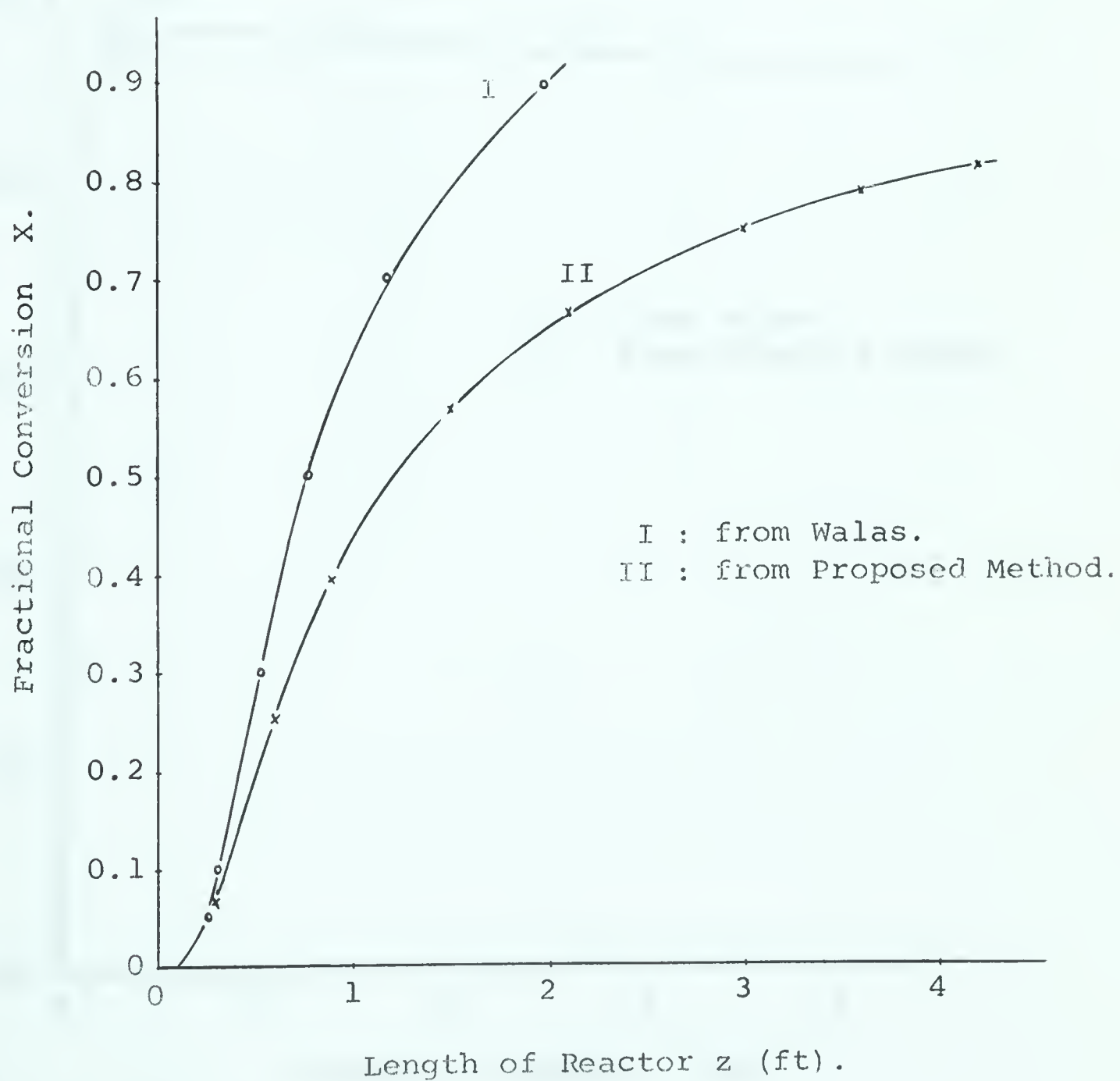
The program was written in Fortran IV and listed in Appendix F.

III.3 Summary

Accurate and stable methods have been proposed for the solution of one-dimensional moving bed reactors, where chemical reaction, if any, occurs only in the gas phase. Finite-difference techniques lead to a set of simultaneous first-order ordinary differential equations, which may then be solved either by using the Runge-Kutta-Gill method on a digital computer or by an analog computer.

Graph 4a

Fractional Conversion Profiles in
Thermal Cracking of n-Butane in Moving Bed Reactor.



Graph 4b

Gas Temperature Profile in
Thermal Cracking of n-Butane.

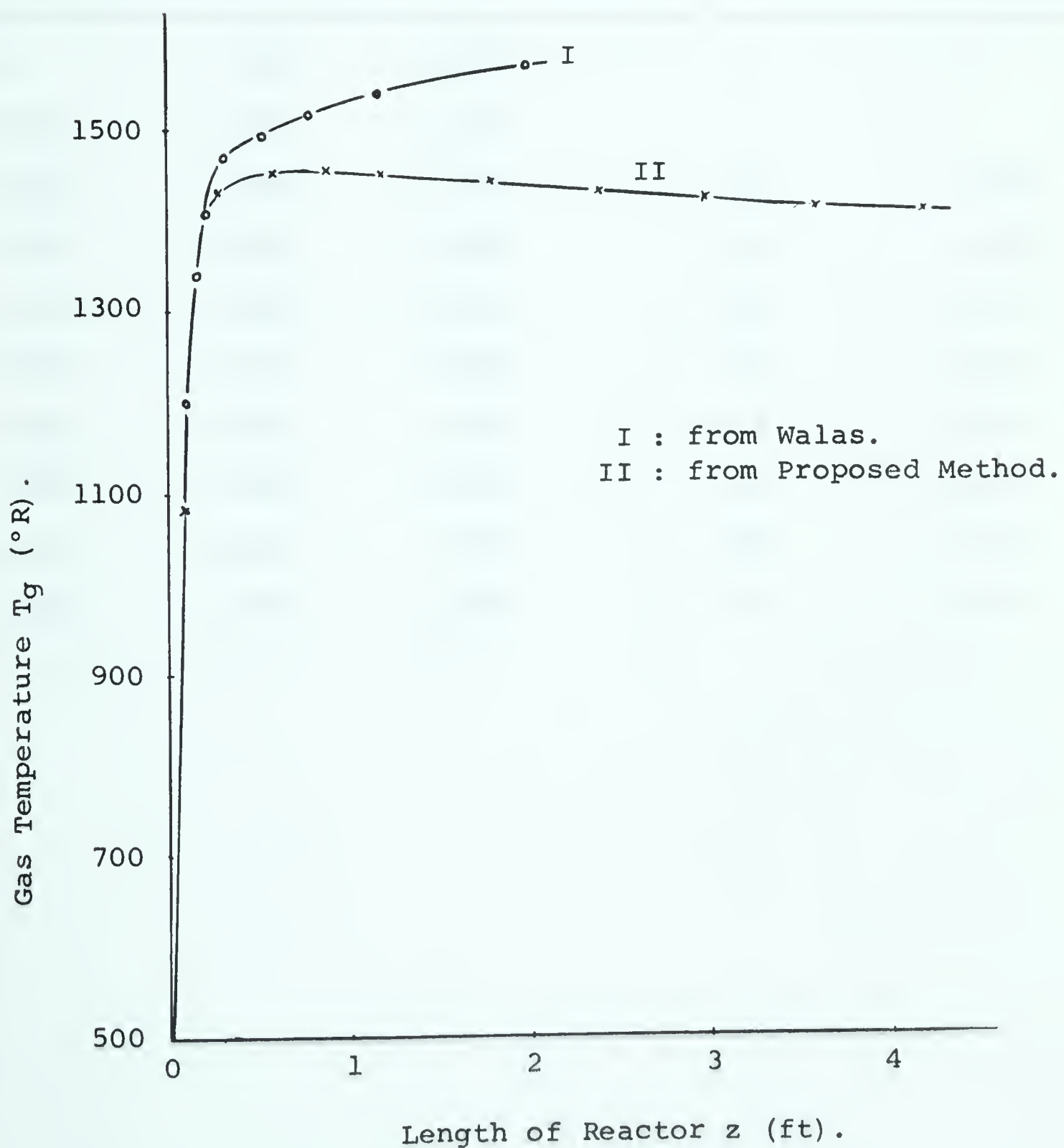


TABLE 4a
Results in Thermal Cracking of
Butane from Walas

Reactor Length (ft)	Gas Temp. (°R)	Solid Temp. (°R)	Temp. Difference (°R)	Conversion
0	500	2000	-	0
0.105	1200	1919	-	0
0.175	1340	1901	561	0.003
0.212	1408	1889	481	0.015
0.259	1464	1874	410	0.05
0.305	1473	1864	391	0.10
0.520	1496	1809	313	0.30
0.792	1520	1756	234	0.50
1.179	1541	1703	162	0.70
1.988	1575	1650	75	0.90

TABLE 4b
Results in Thermal Cracking of
Butane by Proposed Method

Reactor Length (ft)	Gas Temp. (°R)	Surface Temp. (°R)	Temp. Difference (°R)	Conversion
0	500	2000	-	0
0.10	1084.4	1768.9	-	0
0.30	1432.7	1713.1	280.4	0.0663
0.60	1451.4	1640.2	188.8	0.2582
1.20	1452.9	1547.8	94.9	0.4941
1.80	1444.7	1497.7	53.0	0.6229
2.40	1435.0	1467.7	32.7	0.7008
3.00	1426.2	1448.1	21.9	0.7521
3.60	1418.7	1434.4	15.7	0.7883
4.20	1412.4	1424.2	11.8	0.8152
4.80	1407.2	1416.4	9.2	0.8359

Both example problems demonstrate the validity and practicability of the proposed numerical method. From the object times of computation the method can be considered as efficient. The second problem, however, reveals the error of assuming uniform temperature gradients in the solid, which leads to considerable underdesign of the reactor.

IV. FIXED BED REGENERATIVE REACTOR DESIGN

Under the assumptions outlined in the introduction, the reactor may be described mathematically as follows:

1. The energy balance on the fluid contained in a differential volume of the reactor of unit cross-sectional area and length dz is given by

$$\begin{aligned}
 & \epsilon dz \frac{\partial}{\partial z} (T_g \cdot c_f \cdot \rho_f \cdot v_f) + A_s dz \cdot h_f \cdot (T_g - T_s) \\
 & + G_m^o \cdot dz \cdot \sum_{j=1}^N \frac{\partial x_j}{\partial z} \Delta H_j \\
 & = - \epsilon dz \frac{\partial}{\partial t} (\rho_f \cdot c_f \cdot T_g)
 \end{aligned} \tag{IV.1}$$

which simplifies to

$$\begin{aligned}
 & G \frac{\partial}{\partial z} (c_f T_g) + \frac{3(1 - \epsilon) h_f (T_g - T_s)}{R} \\
 & + G_m^o \cdot \sum_{j=1}^N \frac{\partial x_j}{\partial z} \Delta H_j \\
 & = - \epsilon \frac{\partial}{\partial t} (\rho_f c_f T_g)
 \end{aligned} \tag{IV.2}$$

where

$$\frac{\partial x_j}{\partial z} = x_j (x_1, x_2, \dots, x_N, P, T_g) \quad j=1, 2, \dots, N \tag{IV.3}$$

Equation (IV.3) stands for the fractional conversion rate of the j th limiting component in the system of N independent reactions.

2. The pressure drop for^a fixed bed, if considered, is given empirically(14) as

$$\frac{\partial P}{\partial z} = \frac{-G(1 - \epsilon)}{\rho_f g_c D_p \epsilon^3} \cdot \left(\frac{150 (1 - \epsilon) \mu}{D_p} + 1.75G \right) \quad (\text{IV.4})$$

3. The thermal behavior of the individual solid particle is described by

$$c_s \rho_s \frac{\partial T}{\partial t} = k_s \left(\frac{\partial^2 T}{\partial r^2} + \frac{2}{r} \frac{\partial T}{\partial r} \right) \quad (\text{IV.5})$$

Again equations (IV.2) and (IV.5) are coupled by a heat balance at the gas-solid interface.

$$-k_s \left(\frac{\partial T}{\partial r} \right)_{r=R} = h_f (T_s - T_g) \quad (\text{IV.6})$$

The other boundary condition for the solid phase is

$$\frac{\partial T}{\partial r} = 0 \quad \text{at} \quad r = 0 \quad (\text{IV.7})$$

which denotes radial symmetry.

The initial conditions are

$$T_g = T_g(t) \quad \text{at} \quad z = 0 \quad (\text{IV.8})$$

$$T = T(r, z) \quad \text{at} \quad t = \int_0^z \frac{dz}{v_f}$$

Equation (IV.2) is based on a heat balance on a fixed element in space, i.e. Eulerian view point. Alternately, by adopting the more convenient Lagrangian point of view, that is to follow a fixed differential mass of fluid as it proceeds through the reactor, it is possible to eliminate the time variable and reduce equation (IV.2) to an ordinary differential equation. This implies that there is no change in mass of the fluid in passing through the differential element of reactor with time. In terms of the new transformed variable of

$$\theta = t - \int_0^z \frac{dz'}{v_f} \quad (\text{IV.9})$$

the equations describing the system are now

$$\frac{dT_g}{dz} = \frac{3(1 - \epsilon)h_f}{R G c_f} (T_s - T_g) - \frac{G_m^0}{G c_f} \sum_{j=1}^N \frac{dx_j}{dz} \Delta H_j \quad (\text{IV.10})$$

together with equations (IV.3) and (IV.4) for the gas phase;

$$\frac{\partial T}{\partial \theta} = K \left(\frac{\partial^2 T}{\partial r^2} + \frac{2}{r} \frac{\partial T}{\partial r} \right) \quad (\text{IV.11})$$

and the boundary conditions (IV.6) and (IV.7) for the solid.

While the initial conditions are

$$\begin{aligned}
T_g &= T_g(t) \\
x_j &= x_j^0 \quad \text{at } z = 0 \\
P &= P^0
\end{aligned}
\tag{IV.12}$$

and $T = T(r, 0) \quad \theta = 0$

IV.1 Previous Analytical Solutions

A general analytical solution for the above coupled system of differential equations is not available. However, an analytical solution of a simplified case was proposed by Schumann(15). In the absence of chemical reaction in the gas phase and neglecting the temperature gradient in the solid the mathematical model can be reduced to the following

$$\frac{\partial T_g}{\partial t} + v_f \frac{\partial T_g}{\partial z} = \frac{-3(1 - \epsilon) h_f}{\epsilon R c_f \rho_f} (T_g - T) \tag{IV.13}$$

$$\frac{\partial T}{\partial t} = \frac{3h_f}{R c_s \rho_s} (T_g - T) \tag{IV.14}$$

In terms of the new variables, defined below,

$$Y = \frac{3(1 - \epsilon)}{\epsilon R} \cdot \frac{h_f z}{c_f \rho_f v_f} \tag{IV.15}$$

and

$$Z = \frac{3h_f}{R c_s \rho_s} \left(t - \frac{z}{v_f} \right)$$

equations (IV.13) and (IV.14) become

$$\frac{\partial T_g}{\partial Y} = T - T_g \quad (\text{IV.16})$$

$$\frac{\partial T}{\partial Z} = T_g - T \quad (\text{IV.17})$$

with initial conditions

$$T_g = T_g^0 \quad \text{at } Y = 0 \quad (\text{IV.18})$$

$$T = T^0 \quad \text{at } Z = 0.$$

Strictly speaking, the above equations are true only if V_f is constant, but Jakob(16) has shown that for most practical cases, the error introduced by moderate variations in V_f is negligible.

After solving equations (IV.16) and (IV.17) simultaneously with the initial conditions (IV.18), the solution for the gas temperature is

$$\frac{T_g - T^0}{T_g^0 - T^0} = e^{-(Y+Z)} \sum_{n=0}^{\infty} Z^n M_n(YZ) \quad (\text{IV.19})$$

and for the solid temperature is

$$\frac{T - T^0}{T_g^0 - T^0} = e^{-(Y+Z)} \sum_{n=1}^{\infty} Z^n M_n(YZ). \quad (\text{IV.20})$$

In letting $a = ZY$, then

$$\begin{aligned}
 M_0(a) &= 1 + a + \frac{a^2}{(2!)^2} + \frac{a^3}{(3!)^2} + \dots \\
 &= \sum_{i=0}^{\infty} \frac{a^i}{(i!)^2}
 \end{aligned} \tag{IV.21}$$

and

$$M_n(a) = \frac{d^n}{da^n} (M_0(a)).$$

IV.2 Physical Representation of Mathematical Model

The mathematical model proposed for the numerical analysis consists of

1. an elemental volume of reactor of unit cross-section and length Δz , in which the temperature distribution in the solid particle is the same throughout the element.

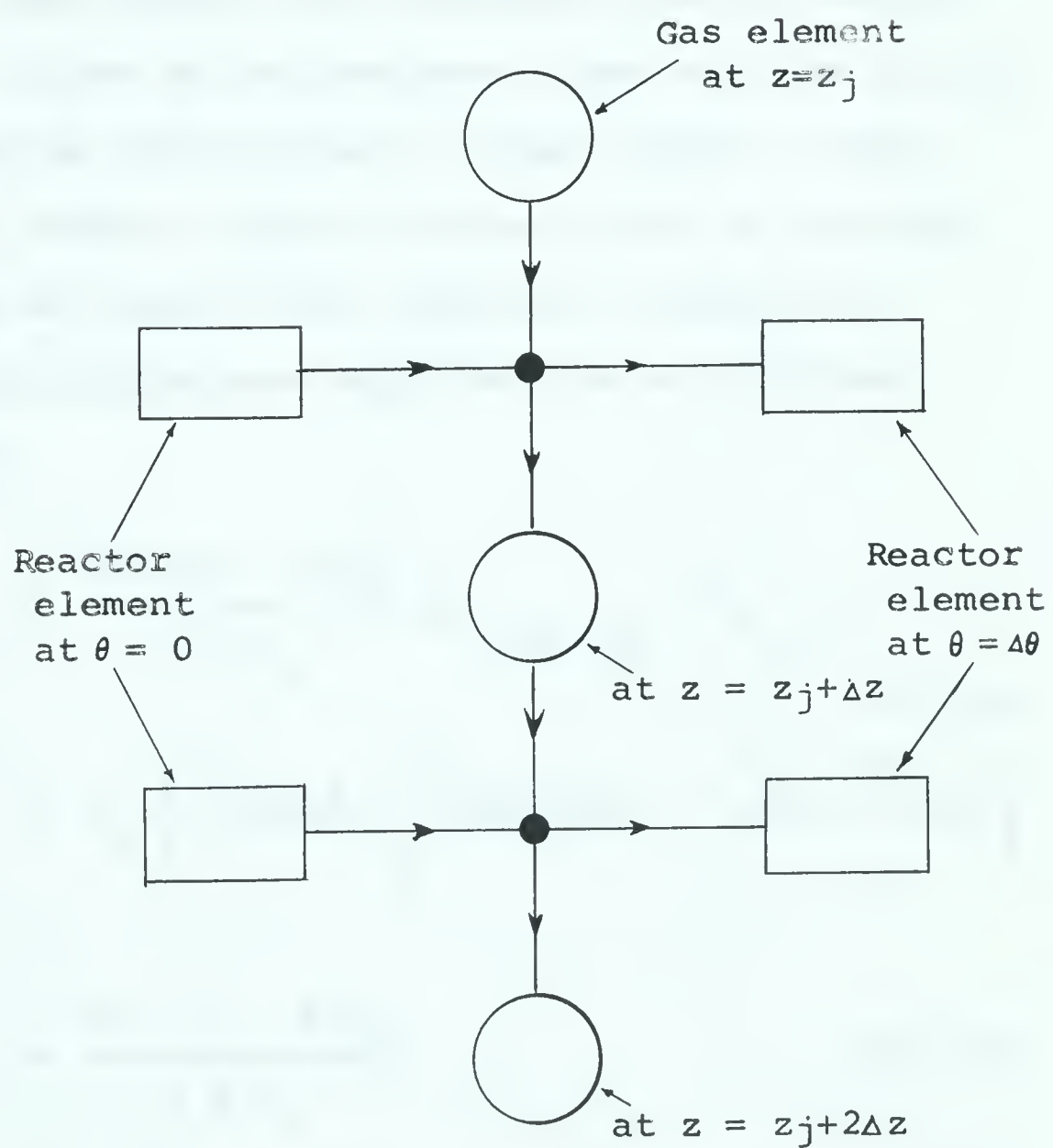
2. an elemental slug of fluid of such size that it would pass through the reactor element in time $\Delta \theta$.

The model merely involves bringing the solid and the fluid into contact at time zero and following the behavior of both over the time interval $\Delta \theta$.

The slug of fluid then goes on to contact the next reactor element and so on through the reactor. In this way the thermal condition of the solid bed is determined for one $\Delta \theta$. The procedure is then repeated for the next slug of fluid.

Figure 3

Diagrammatical Representation of
the Mathematical Model for the
Regenerative Bed Reactor.



Intersections may be considered to be stirred tanks.

It should be noted that in the following calculations, the time average is used for the solid surface temperature and position average for the gas temperature. In fact, the model reduces to a series of stirred tank calculations. Diagrammatically it is illustrated in Figure 3.

IV.3 The Fixed Bed Regenerative Heat Exchanger

In this case, there is no chemical reaction and if the pressure drop is not to be considered then equation (IV.10) together with equation (IV.11) form a linear system. That means a completely stable, implicit method, such as outlined in Section II, can be used for the numerical integration.

The finite-difference approximation of equation (IV.10) is given by

$$\begin{aligned}
 T_{g_{i+1}} - T_{g_i} &= \frac{\Delta z \cdot 3(1 - \epsilon) h_f}{R G c_f} (T_{s_{j+\frac{1}{2}, i+\frac{1}{2}}} - T_{g_{i+\frac{1}{2}}}) \\
 &= A_1 \left\{ \frac{T_{s_{j+\frac{1}{2}, i}} + T_{s_{j+\frac{1}{2}, i+1}}}{2} - \frac{T_{g_i} + T_{g_{i+1}}}{2} \right\}
 \end{aligned} \tag{IV.22}$$

where

$$A_1 = \frac{\Delta z \cdot 3(1 - \epsilon) h_f}{R G c_f} \tag{IV.23}$$

In the above equations the subscript j is used to denote reactor position and the subscript i to denote time.

Thus, the solid surface temperature is at the time average and the gas temperature at the position average as described in the model.

For the solid phase, the partial differential equation (IV.11) is replaced by a set of ordinary differential equations, listed in Table 3, with the radius being divided into 5 equal lengths and the temperature at the center of each length representing the mean temperature of the spherical shell. Expressing equations (IV.22) and (IV.11) in Crank-Nicholson implicit form, the computational system becomes:

$$\begin{aligned}
 & \left(1 + \frac{13B}{8}\right)T_{1,i+1} - \left(\frac{27B}{16}\right)T_{2,i+1} + \left(\frac{B}{16}\right)T_{3,i+1} \\
 &= \left(1 - \frac{13B}{8}\right)T_{1,i} + \left(\frac{27B}{16}\right)T_{2,i} - \left(\frac{B}{16}\right)T_{3,i} \\
 & \quad \left(\frac{B}{18}\right)T_{1,i+1} + \left(1 + \frac{2B}{3}\right)T_{2,i+1} - \left(\frac{13B}{8}\right)T_{3,i+1} \\
 &= -\left(\frac{B}{18}\right)T_{1,i} + \left(1 - \frac{2B}{3}\right)T_{2,i} + \left(\frac{13B}{8}\right)T_{3,i} \\
 & - \left(\frac{B}{15}\right)T_{1,i+1} - \left(\frac{B}{10}\right)T_{2,i+1} + \left(1 + \frac{4B}{5}\right)T_{3,i+1} - \left(\frac{19B}{30}\right)T_{4,i+1} \\
 &= \left(\frac{B}{15}\right)T_{1,i} + \left(\frac{B}{10}\right)T_{2,i} + \left(1 - \frac{4B}{5}\right)T_{3,i} + \left(\frac{19B}{30}\right)T_{4,i}
 \end{aligned}$$

$$\begin{aligned}
& - \left(\frac{B}{21}\right) T_{2,i+1} - \left(\frac{3B}{14}\right) T_{3,i+1} + \left(1 + \frac{6B}{7}\right) T_{4,i+1} - \left(\frac{25B}{42}\right) T_{5,i+1} \\
& = \left(\frac{B}{21}\right) T_{2,i} + \left(\frac{3B}{14}\right) T_{3,i} + \left(1 - \frac{6B}{7}\right) T_{4,i} + \left(\frac{25B}{42}\right) T_{5,i} \\
& (42 - 9\gamma) T_{3,i+1} + (50\gamma - 460) T_{4,i+1} + \left(\frac{540}{B} + 1410 - 225\gamma\right) T_{5,i+1} \\
& - \gamma\beta T_{g_{j+1}}
\end{aligned} \tag{IV.24}$$

$$\begin{aligned}
& = (9\gamma - 42) T_{3,i} + (460 - 50\gamma) T_{4,i} + \left(\frac{540}{B} - 1410 + 225\gamma\right) T_{5,i} \\
& + \gamma\beta T_{g_i}
\end{aligned}$$

$$\begin{aligned}
& - 9T_{3,i+1} + 50T_{4,i+1} - 225T_{5,i+1} + (184 + 2(184 + \beta)/A_1) T_{g_{j+1}} \\
& = 9T_{3,i} - 50T_{4,i} + 225T_{5,i} - (184 - 2(184 + \beta)/A_1) T_{g_j}
\end{aligned}$$

where

$$\Delta r = R/5$$

$$B = \Delta\theta K / \Delta r^2$$

$$\beta = 60\Delta r h_f / k_s$$

$$\gamma = 992 / (184 + \beta)$$

It should be noted that all the terms in equation (III.11) are third order correct. A system of second order correct expressions had been tried but this led to unsatisfactory results. The system of equations (IV.24) is, in fact, a set of simultaneous linear algebraic equations which can be written algebraically as in Table 5. The coefficient matrix can be transformed by simple arithmetic operations into a tridiagonal matrix, which can then be readily solved by the Thomas method(17).

A numerical problem was solved to check the feasibility of the implicit method against the analytical solution by Schumann for a system with negligible intraparticle temperature gradients.

IV.4 The Regenerative Bed Fluid Phase Reactor

The presence of non-linear terms, as a result of chemical reaction in equation (IV.10), make difficult if not outright impractical the implicit method outlined in the preceding section. Thus, resource to some kind of explicit method operating on equation (IV.10) seems logical. However, the stability of these methods depends upon the magnitude of the term $(K\Delta\theta/\Delta r^2)$, which cannot exceed some limiting value. This value cannot be easily predicted for systems of non-linear differential equations and depends on the very nature of the non-linear terms. Usually, in order to preserve stability, $\Delta\theta$ has to be made so small that an extraordinarily large number of time steps must be used to obtain a practical solution.

TABLE 5

The Simultaneous Linear Algebraic Form of Equations
for Fixed Bed Regenerative Heat Exchanger

$$\begin{bmatrix}
 a_{11} & a_{12} & a_{13} & & & \\
 a_{21} & a_{22} & a_{23} & & & \\
 a_{31} & a_{32} & a_{33} & a_{34} & & \\
 & a_{42} & a_{43} & a_{44} & a_{45} & \\
 & & a_{53} & a_{54} & a_{55} & a_{56} \\
 & & a_{63} & a_{64} & a_{65} & a_{66}
 \end{bmatrix}
 \begin{bmatrix}
 T_{1,i+1} \\
 T_{2,i+1} \\
 T_{3,i+1} \\
 T_{4,i+1} \\
 T_{5,i+1} \\
 T_{6,i+1}
 \end{bmatrix}
 =
 \begin{bmatrix}
 b_1 \\
 b_2 \\
 b_3 \\
 b_4 \\
 b_5 \\
 b_6
 \end{bmatrix}$$

where

$$T_{6,i+1} = T_{g_{j+1}}$$

$$b_k = b_k (T_{1,i}, T_{2,i}, \dots, T_{5,i}, T_{g_j})$$

$$k = 1, 2, \dots, 6$$

It is proposed here that the problem can be reduced to manageable proportions by decoupling the two phases. In principle, the method involves substituting an explicit function for T_s in terms of θ in place of the coupling boundary condition given by equation (IV.6). As a first approximation, it is assumed that over a short time increment the surface temperature changes linearly with time, i.e.

$$T_s = T_s^o + q \theta \quad (\text{IV.25})$$

where the superscript "o" signifies the beginning of the time increment and q is some constant to be determined. According to the model, the elemental slug of fluid will see a constant solid surface temperature of $(T_s^o + q\Delta\theta/2)$.

Thus, the correct value of q is that which will equate Q_s the total heat gained by the solid phase in time $\Delta\theta$ and Q_g the enthalpy lost by the elemental slug of fluid under consideration. To evaluate these quantities, equations (IV.3), (IV.4), (IV.10) and (IV.11) have to be solved for the assumed boundary condition.

The solid phase will be considered first. Since equation (IV.11) is linear, the principle of superposition can be applied; hence, it can be replaced by two other systems, each with simpler boundary conditions. Let

$$T = u + w \quad (\text{IV.26})$$

Then

$$\frac{\partial w}{\partial \theta} = K \left(\frac{\partial^2 w}{\partial r^2} + \frac{2}{r} \frac{\partial w}{\partial r} \right) \quad (\text{IV.27})$$

with boundary conditions

$$\frac{\partial w}{\partial r} = 0 \quad \text{at } r = 0 \quad (\text{IV.28a})$$

$$w = T_s^0 + q \theta \quad \text{at } r = R \quad (\text{IV.28b})$$

and initial condition

$$w = 0 \quad \theta = 0 \quad (\text{IV.28c})$$

Also

$$\frac{\partial u}{\partial \theta} = K \left(\frac{\partial^2 u}{\partial r^2} + \frac{2}{r} \frac{\partial u}{\partial r} \right) \quad (\text{IV.29})$$

with boundary conditions

$$\frac{\partial u}{\partial r} = 0 \quad r = 0 \quad (\text{IV.30a})$$

$$u = 0 \quad r = R \quad (\text{IV.30b})$$

and initial condition

$$u = T(r) \quad \theta = 0 \quad (\text{IV.30c})$$

Equation (IV.27) with its associated boundary conditions can readily be solved by applying the Laplace transformation to obtain a series solution involving the error function as follows:

$$W = \frac{RT_s^0}{r} \sum_{n=0}^{\infty} \left\{ \operatorname{erfc} \left(\frac{\gamma_n}{\lambda} \right) - \operatorname{erfc} \left(\frac{\delta_n}{\lambda} \right) \right\}$$

$$\begin{aligned}
& + \frac{Rq}{r} \sum_{n=0}^{\infty} \left\{ \left[\left(\Theta + \frac{\gamma_n^2}{2K} \right) \operatorname{erfc} \left(\frac{\gamma_n}{\lambda} \right) - \gamma_n \left(\frac{\Theta}{\pi K} \right)^{1/2} \exp \left(-\left(\frac{\gamma_n}{\lambda} \right)^2 \right) \right] \right. \\
& \left. - \left[\left(\Theta + \frac{\delta_n^2}{2K} \right) \operatorname{erfc} \left(\frac{\delta_n}{\lambda} \right) - \delta_n \left(\frac{\Theta}{\pi K} \right)^{1/2} \exp \left(-\left(\frac{\delta_n}{\lambda} \right)^2 \right) \right] \right\} \quad (\text{IV.31})
\end{aligned}$$

where

$$\begin{aligned}
\gamma_n &= (2n + 1) R - r \\
\lambda &= 2(K\Theta)^{1/2} \\
\delta_n &= (2n + 1) R + r
\end{aligned}$$

Equation (IV.29) with its associated boundary conditions is usually handled by the method of separation of variables with the initial condition in discrete form. Expansion into an infinite series of orthogonal functions, results in

$$u = \frac{2}{Rr} \sum_{n=1}^{\infty} \exp(-K\alpha_n^2 \Theta) \cdot \sin \alpha_n r \cdot \int_0^R r' T(r') \cdot \sin \alpha_n r' \cdot dr' \quad (\text{IV.32})$$

where

$$\alpha_n = n\pi/R$$

However, practical computational problems arise since the series which gives the heat content change over a small interval of time $\Delta\Theta$, as shown below,

$$\int_0^{\Delta\theta} \left(\frac{\partial u}{\partial r}\right)_{r=R} d\theta = \frac{2}{KR\pi} \sum_{n=1}^{\infty} \frac{(-1)^n}{n} \left\{ 1 - \exp\left(-\frac{Kn^2\pi^2\Delta\theta}{R^2}\right) \right\}$$

$$\int_0^R r' T(r') \sin \frac{n\pi r'}{R} dr' \quad (\text{IV.33})$$

converges very slowly due to the smallness of the quantity $(Kn^2\pi^2\Delta\theta/R^2)$.

To resolve this difficulty, Green's function for an instantaneous spherical surface source is used. For an infinite sphere the temperature at r , due to an instantaneous spherical surface source of strength Q' at $\theta = 0$ and of radius r' , is given(18) as

$$u_1 = \frac{Q'}{8\pi r r' (\pi K \theta)^{1/2}} \left\{ \exp\left(\frac{-(r - r')^2}{4K\theta}\right) - \exp\left(\frac{-(r + r')^2}{4K\theta}\right) \right\} \quad (\text{IV.34})$$

Now for a finite sphere with unit instantaneous spherical surface source at $\theta = 0$ and of radius r' the temperature is given by u' , such that

$$u' = u_1 + u_2 \quad (\text{IV.35})$$

where u_2 vanished at $\theta = 0$ and is such that u' satisfies

$$\frac{\partial u'}{\partial \theta} = K \left(\frac{\partial^2 u'}{\partial r^2} + \frac{2}{r} \frac{\partial u'}{\partial r} \right) \quad (\text{IV.36})$$

with

$$u' = \text{unit inst. source} \quad \theta = 0$$

$$u' = 0 \quad r = R$$

$$\frac{\partial u'}{\partial r} = 0 \quad r = 0$$

Since u_2 also satisfies the heat conduction equation,

$$\frac{\partial^2 (ru_2)}{\partial r^2} - \frac{1}{K} \frac{\partial (ru_2)}{\partial \theta} = 0 \quad (\text{IV.37})$$

Taking the Laplace transformation with respect to θ , (IV.37) becomes

$$\frac{d^2 (r\bar{u}_2)}{dr^2} - q^2 (r\bar{u}_2) = 0 \quad (\text{IV.38})$$

where

$$\bar{u}_2 = \int_0^\infty e^{-p\theta} u_2 d\theta$$

$$q^2 = p/K.$$

The general solution of equation (IV.38) is

$$\bar{u}_2 = \frac{1}{r} (c_1 \sinh qr + c_2 \cosh qr). \quad (\text{IV.39})$$

At $r = 0$, \bar{u}_2 is finite, so $c_2 = 0$

However, at $r = R$

$$\bar{u}' = \bar{u}_1 + \bar{u}_2 = 0$$

Therefore,

$$\begin{aligned}\bar{u}_1 + \bar{u}_2 &= \frac{1}{8\pi R r' K q} \left\{ \exp(-q(R - r')) \right. \\ &\quad \left. - \exp(-q(R + r')) \right\} + c_1 (\sinh qR)/R \\ &= 0\end{aligned}$$

where Q' is unity.

After solving for c_1 and back substituting into \bar{u}' , it gives

$$\bar{u}' = \frac{\sinh qr \cdot \sinh q(R - r')}{4\pi r r' K q \sinh qR} \quad (\text{IV.40})$$

Expanding in a series of negative exponentials and taking the back transformation from tables, the solution is

$$\begin{aligned}u' &= \frac{1}{8rr'\pi(\pi K\theta)^{1/2}} \sum_{n=-\infty}^{\infty} \left\{ \exp \left[-\frac{(2nR - r + r')^2}{4K\theta} \right] \right. \\ &\quad \left. - \exp \left[-\frac{(2nR + r + r')^2}{4K\theta} \right] \right\} \quad (\text{IV.41})\end{aligned}$$

If now the initial condition for u is considered, i.e. of source strength $4\pi(r')^2 T(r')dr'$ on the sphere at r'

$$u = \frac{1}{2r(\pi K\theta)^{1/2}} \sum_{n=-\infty}^{\infty} \int_0^R r' T(r') \left\{ \exp \left[-\frac{(2nR - r + r')^2}{4K\theta} \right] - \exp \left[-\frac{(2nR + r + r')^2}{4K\theta} \right] \right\} dr' \quad (\text{IV.42})$$

In essence, the Green's function permits the evaluation of the temperature at any point due to an instantaneous surface source which moves from the centre to the outer boundary. Mathematically this is equivalent to calculating the additive component of temperature due to the initial temperature distribution within the particle.

Thus, the solid temperature T is obtained simply by adding equations (IV.31) and (IV.42), that is

$$T = \frac{1}{2r(\pi K\theta)^{1/2}} \sum_{n=-\infty}^{\infty} \int_0^R r' T(r') \left\{ \exp \left[\frac{-(2nR - r + r')^2}{4K\theta} \right] - \exp \left[\frac{-(2nR + r + r')^2}{4K\theta} \right] \right\} dr' + \frac{RT_s^0}{r} \sum_{n=0}^{\infty} \left\{ \operatorname{erfc} \left(\frac{\gamma_n}{\lambda} \right) - \operatorname{erfc} \left(\frac{\delta_n}{\lambda} \right) \right\}$$

$$\begin{aligned}
& + \frac{Rq}{r} \sum_{n=0}^{\infty} \left\{ \left[\left(\Theta + \frac{\gamma_n^2}{2K} \right) \operatorname{erfc} \left(\frac{\gamma_n}{\lambda} \right) - \gamma_n \left(\frac{\Theta}{\pi K} \right)^{\frac{1}{2}} \exp \left(- \left(\frac{\gamma_n}{\lambda} \right)^2 \right) \right] \right. \\
& \left. - \left[\left(\Theta + \frac{\delta_n^2}{2K} \right) \operatorname{erfc} \left(\frac{\delta_n}{\lambda} \right) - \delta_n \left(\frac{\Theta}{\pi K} \right)^{\frac{1}{2}} \exp \left(- \left(\frac{\delta_n}{\lambda} \right)^2 \right) \right] \right\} \quad (\text{IV.43})
\end{aligned}$$

where

$$\begin{aligned}
\gamma_n &= (2n + 1) R - r & \delta_n &= (2n + 1) R + r \\
\lambda &= 2(K\Theta)^{\frac{1}{2}}
\end{aligned}$$

It is not difficult, though tedious, to verify that this solution indeed satisfies the heat conduction equation and the associated boundary conditions. However, it is proved in Appendix E, that it satisfies the initial condition $T(r)$.

Now the total heat content change Q_s of the solid over the time interval $\Delta\Theta$ can be calculated by integrating the temperature distribution thus obtained over the whole volume of the particle. However, this would have to be repeated for each new value of q .

A more efficient method is to evaluate the heat flux at the surface and integrate this over the time interval.

$$Q_s = \frac{3(1 - \epsilon) \Delta z}{R} \int_0^{\Delta\Theta} k_s \left(\frac{\partial T}{\partial r} \right)_{r=R} d\Theta$$

$$\begin{aligned}
= & \frac{3(1 - \epsilon)\Delta z k_s}{R} \left\{ \sum_{n=0}^{\infty} \frac{1}{KR} \int_0^R r' T(r') \left[\operatorname{erfc} \left(\frac{2nR + R + r'}{2\sqrt{K\Delta\theta}} \right) \right. \right. \\
& - \left. \operatorname{erfc} \left(\frac{2nR + R - r'}{2\sqrt{K\Delta\theta}} \right) \right] dr' + T_s^o \left[\frac{-\Delta\theta}{R} + 2\sqrt{\frac{\Delta\theta}{K\pi}} \right] \\
& + q \left[\frac{-\Delta\theta^2}{2R} + \frac{4}{3}\sqrt{\frac{\Delta\theta^3}{K\pi}} \right] + 2T_s^o \sum_{n=1}^{\infty} \left[2\sqrt{\frac{\Delta\theta}{K\pi}} \exp \left(-\frac{n^2 R^2}{K\Delta\theta} \right) \right. \\
& - \left. \frac{2nR}{K} \operatorname{erfc} \left(\frac{nR}{\sqrt{K\Delta\theta}} \right) \right] - \frac{8R^3 q}{K^2} \sum_{n=1}^{\infty} \left[\frac{K\Delta\theta n}{2R^2} \operatorname{erfc} \left(\frac{nR}{\sqrt{K\Delta\theta}} \right) \right. \\
& - \left. \left[\sqrt{\frac{\Delta\theta}{K\pi}} \frac{K}{R} n^2 \exp \left(\frac{-n^2 R^2}{K\Delta\theta} \right) + n^3 \operatorname{erfc} \left(\frac{nR}{\sqrt{K\Delta\theta}} \right) \right] \right] \\
& + \frac{16q R^3}{3K^2 \sqrt{\pi}} \sum_{n=1}^{\infty} n^3 \left[\operatorname{erfc} \left(\frac{nR}{\sqrt{K\Delta\theta}} \right) \cdot \sqrt{\pi} \right. \\
& - \left. \frac{\sqrt{\Delta\theta K}}{nR} \exp \left(\frac{-n^2 R^2}{\Delta\theta K} \right) \left(1 - \frac{\Delta\theta K}{2n^2 R^2} \right) \right] \left. \right\} \quad (\text{IV.44})
\end{aligned}$$

This may be simplified to the form

$$Q_s = A_2 (A_3 + A_4 T_s^o + A_5 q) \quad (\text{IV.45})$$

A_2 , A_4 , A_5 are constants throughout for a given system with fixed Δz and $\Delta\theta$. A_3 and T_s^o are constants that are applicable for each reactor element calculation.

Fortunately, the evaluation of these constants is simplified by the fact that the series given in equation (IV.44) converges very quickly and in practical cases only the first two terms need be considered. It is important to note that the constants need be calculated only once; from then on Q_s can be evaluated for a series of values of q very simply. In this later numerical computation, the integration was performed numerically by Simpson's Rule with error correction(19). The evaluation of the error cofunction is outlined in Appendix E.

The behavior of the gas phase is described by a set of first order ordinary differential equations, using a time-average value of the solid surface temperature as the boundary condition. Thus,

$$\begin{aligned} \frac{dT_g}{dz} = & \frac{3(1 - \epsilon) h_f}{R G c_f} \left(T_s^o + \frac{q\Delta\theta}{2} - T_g \right) \\ & - \frac{G_m^o}{G c_f} \cdot \sum_{j=1}^N \frac{dx_j}{dz} \Delta H_j \end{aligned} \quad (\text{IV.46})$$

together with the above equations (IV.3), (IV.4) and the appropriate initial conditions in equation (IV.12) form an independent system. The enthalpy change may be written as

$$Q_g = G_m^o \cdot \Delta\theta \left\{ (T_{g1} \bar{c}_{p1} - T_{g2} \bar{c}_{g2}) + \sum_{j=1}^N \Delta x_j \Delta H_j \right\} \quad (\text{IV.47})$$

where τ_{p_1} and \bar{c}_{p_2} are the average molar heat capacities of gases at T_{g_1} and T_{g_2} , the initial and final temperature, respectively

IV.5 Computational Results

In setting up a computational model it is generally desirable to proceed in a stepwise fashion - trying at every stage to compare the results either with a known analytical solution, or if that is not possible, with a numerical solution involving techniques that have been tested and shown to be valid and accurate.

IV.5.1 Example Problem No. 1

Consider a reactor packed with copper spheres of radius 0.05 ft. to be used as a heat exchanger in an air liquifaction system. It is desired to calculate the temperature of the air and of the spheres in the exchanger as a function of position and time, under the following operating conditions:

G	$=$	2000 lb/(sq.ft.)(hr)	air flow rate
L	$=$	4.68 ft.	reactor length
T^o	$=$	280 °R	initial temp. of solids
T_g^o	$=$	350 °R	entering air temp.
ϵ	$=$	0.345	fractional voids
h_f	$=$	20 BTU/(hr)(sq.ft.)(°R)	convective heat transfer coefficient
c_f	$=$	0.23 BTU/(lb)(°R)	air heat capacity
ρ_f^o	$=$	23 lb/(cu.ft.)	entering air density

This problem was taken in part from "Applied Mathematics in Chemical Engineering"(20) and was solved for four different cases.

Case 1: The results of the analytical solution by equation (IV.19) for the gas phase, predicated upon a uniform particle temperature are given in Table 6a.

Case 2: The results of the implicit Crank-Nicholson method, outlined in Section IV.3, using a value for K of 5.4 sq.ft./hr. and for k_s of 200 BTU/(hr.ft.)(°R) are also shown in Table 6a. It is expected that the two solutions would be almost identical, since with a high thermal conductivity, (in fact copper was used), the interior particle temperature gradients would be negligible. This can be seen in Table 6b. The close agreement confirms the validity of the numerical method and the accuracy of the finite difference expressions used.

Case 3: The problem was redone, using a K of 0.0106 sq.ft./hr. and k_s of 0.19 BTU/(hr)(°R)(ft), values typical of refractory materials. These were so chosen that significant temperature gradients in the solid particles would exist. The results of the implicit method are tabulated in Table 7 for the gas phase and plotted in Graph No. 5 for the solid phase.

Case 4: The decoupling technique, by solving the solid phase and fluid phase equations separately, was then applied to the problem presented in Case 3. The results of the gas temperature are also listed in Table 7; but the solid temperature gradients are plotted in Graph No. 5. It should be noted that in the program

TABLE 6aGas Temperature Along Fixed Bed AirLiquifaction Heat Exchanger

(negligible intraparticle temperature gradients)

Distance from Entrance (ft)	Gas Temp (°R) at Time θ		
	Analytical Solution	Implicit Method $\Delta\theta=5$ sec	Implicit Method $\Delta\theta = 10$ sec
<u>$\theta = 100$ sec.</u>			
0	350.00	350.00	350.00
0.267	337.40	337.20	336.96
0.609	321.10	320.70	320.31
1.204	305.04	304.43	304.03
1.872	292.73	291.95	291.67
2.675	285.32	284.58	284.43
3.611	281.82	281.29	281.23
4.680	280.50	280.22	280.20
<u>$\theta = 160$ sec.</u>			
0	350.00	350.00	350.00
0.267	341.80	341.72	341.57
0.609	328.95	328.78	328.49
1.204	313.63	313.31	312.96
1.872	299.53	298.99	298.69
2.675	289.43	288.71	288.51
3.611	283.73	283.05	282.96
4.680	281.20	280.73	280.70

TABLE 6bSolid Temperature in Fixed Bed Air LiquifactionHeat Exchange

(negligible intraparticle temperature gradients)

Distance from Entrance (ft)	Solid Temperature (°R) at 160 sec. by Implicit Method				
	T ₁	T ₂	T ₃	T ₄	T ₅
0.1337	328.12	328.13	328.14	328.15	328.15
0.4680	316.74	316.75	316.76	316.77	316.78
0.9360	304.46	304.46	304.47	304.48	304.49
1.5377	293.86	293.86	293.87	293.88	293.88
2.2731	286.49	286.50	265.50	265.50	265.51
3.1423	282.42	282.42	284.42	284.42	284.42
4.1451	280.65	280.65	280.65	280.65	280.65

TABLE 7
Gas Temperature Profile Along
Fixed Bed Heat Exchange

(significant intraparticle temperature gradients)

At time = 5/6 min. at the 8th increment

Fractional Distance From Entrance	Gas Temp. (°R)		
	Decoupling Method with (E = 0.01)	Implicit Method	Simplified Analytic Method
0	350.0	350.0	350.0
1/13	338.10	337.93	333.71
2/13	327.56	327.29	319.80
3/13	318.45	318.11	308.73
4/13	310.76	310.40	300.31
5/13	304.37	304.02	294.12
6/13	299.14	298.83	289.68
7/13	294.92	294.65	286.56
8/13	291.55	291.32	284.40
9/13	288.88	288.70	282.93
10/13	286.78	286.64	281.93
11/13	285.15	285.05	281.26
12/13	283.89	283.82	280.82
13/13	282.45	282.87	280.53

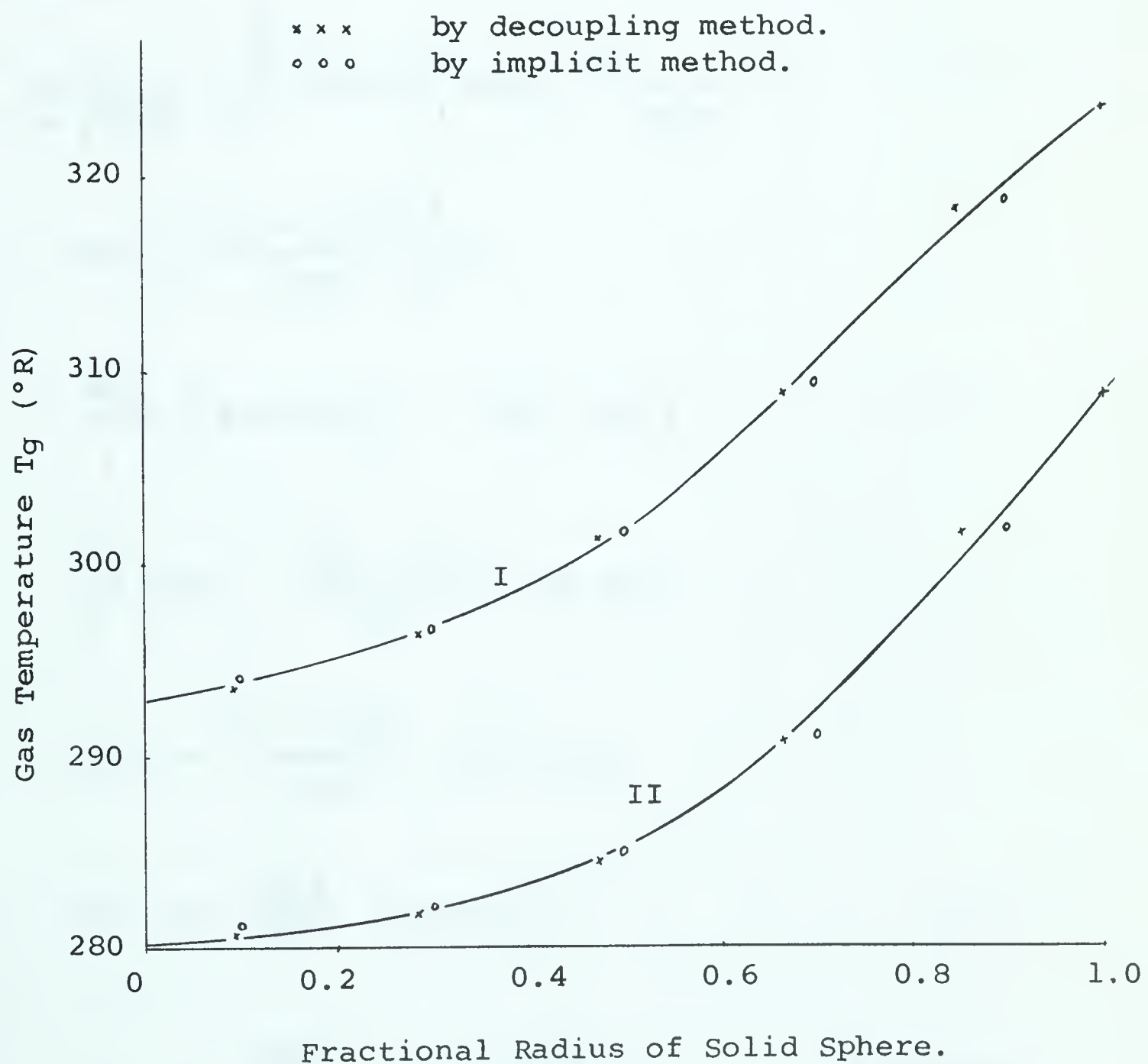
where $E = |Q_s - Q_G| / |Q_s + Q_G|$

Graph No. 5Temperature Gradients in Solids ofRegenerative Bed Heat Exchanger.

(at 1.08 ft from inlet)

I : at time = 2.0833 min.

II : at time = 0.8333 min.



$$\Delta\theta = 0.001736 \text{ (hr)} \quad (1/48 \text{ of } 5 \text{ min. cycle})$$

so

$$\left(\frac{\Delta\theta}{K\pi}\right)^{1/2} = 0.234$$

and

$$\frac{R}{\sqrt{K\Delta\theta}} = 11.7025$$

hence, equations (IV.43) and (IV.44), with the significant terms remaining become

$$\begin{aligned} T = & \frac{1}{2r \sqrt{\pi\Delta\theta K}} \int_0^R r' T(r') \left\{ \exp \left[\frac{-(r - r')^2}{4\Delta\theta K} \right] \right. \\ & - \exp \left[\frac{-(r + r')^2}{4\Delta\theta K} \right] \left. \right\} dr' \\ & + \frac{RT_s^0}{r} \left\{ \operatorname{erfc}(\gamma_0) - \operatorname{erfc}(\delta_0) \right\} \\ & + \frac{Rq}{r} \left\{ \left(\Delta\theta + \frac{(R - r)^2}{2K} \right) \operatorname{erfc}(\gamma_0) \right. \\ & - \left(\Delta\theta + \frac{(R + r)^2}{2K} \right) \operatorname{erfc}(\delta_0) \\ & - (R - r) \left(\frac{\Delta\theta}{\pi K} \right)^{1/2} \exp(-\gamma_0^2) \\ & + \left. (R + r) \left(\frac{\Delta\theta}{\pi K} \right)^{1/2} \exp(-\delta_0^2) \right\} \end{aligned} \quad (\text{IV.48})$$

and

$$\begin{aligned}
 Q_s &= A_2 (A_3 + A_4 T_s^0 + A_5 q) \\
 &= \frac{3\Delta z(1 - \epsilon)k_s}{R} \left\{ \int_0^R \frac{rT(r')}{KR} \left[\operatorname{erfc}(\delta_0) - \operatorname{erfc}(\gamma_0) \right] dr' \right. \\
 &\quad + p \left[\frac{-\Delta\theta}{R} + 2 \left(\frac{\Delta\theta}{\pi K} \right)^{1/2} \right] \\
 &\quad \left. + q \left[\frac{-\Delta\theta^2}{2R} + \frac{4\Delta\theta}{3} \left(\frac{\Delta\theta}{\pi K} \right)^{1/2} \right] \right\} \quad (\text{IV.49})
 \end{aligned}$$

where

$$\begin{aligned}
 \gamma_0 &= (R - r)/2 \sqrt{\Delta\theta K} \\
 \delta_0 &= (R + r)/2 \sqrt{\Delta\theta K}
 \end{aligned}$$

For equation (IV.48) the temperature consists of three components, namely, of initial temperature distribution $T(r)$, of constant surface temperature T_s^0 and of rate of change of temperature q . Due to the presence of exponential terms, the numerical integration will not give satisfactory results unless the radius is divided into more than 15 sections. However, the accuracy of this expression is demonstrated in Table 8.

If T_{g1} and T_{g2} are the gas temperatures at the beginning and ending of Δz section of the bed, then the total heat content change in the gas phase for time interval $\Delta\theta$ is

$$Q_G = (T_{g1} - T_{g2}) \Delta\theta \epsilon c_f G \quad (\text{IV.50})$$

TABLE 8

Temperature of Solid by Equation (IV.48)

$$\text{at } T(r') = 280 \text{ (}^\circ\text{R)}$$

$$T_s^o = 280 \text{ (}^\circ\text{R)}$$

$$q = 0 \text{ (}^\circ\text{R/hr)}$$

as a check on equation (IV.42)

r	Temp. due to $T(r)$	Temp. due to T_s^o	Final $T(r)$
R/20	279.915	0.000	279.92
R/10	279.991	0.000	279.99
2R/10	279.983	0.000	279.98
3R/10	279.991	0.000	279.99
4R/10	280.008	0.000	280.01
5R/10	279.971	0.020	279.99
6R/10	279.572	0.436	280.01
7R/10	274.772	5.220	279.99
8R/10	245.744	34.278	280.02
9R/10	153.049	126.924	279.97
R	1.3×10^{-14}	280.00	280.00

The calculation procedure may be stated as follows:

1. estimate the surface temperature from equation (IV.6) so

$$T_s = \frac{\left(\frac{12\Delta r h_f}{k_s}\right) T_{g1} + 18T_n - 9T_{n-1} + 2T_{n-2}}{\left(11 + \frac{12 \Delta r h_f}{k_s}\right)} \quad (\text{IV.51})$$

where T_n is the outermost solid temperature.

2. obtain q as a first approximation

$$q = \frac{T_s - T_s^o}{\Delta\theta}$$

3. calculate Q_s from equation (IV.49)
4. solve equation (IV.46) with reaction term neglected to get T_{g2}
5. calculate Q_g from equation (IV.50)
6. if $|Q_s - Q_g| \leq \lambda$, a given allowable difference proceed to another increment and repeat the whole process of computation,
7. if $|Q_s - Q_g| > \lambda$, find a new q from

$$q = \frac{\frac{(Q_s + Q_g)}{2} - A_2 A_3 - A_2 A_4 T_s^o}{A_2 A_5} \quad (\text{IV.52})$$

and go to 3.

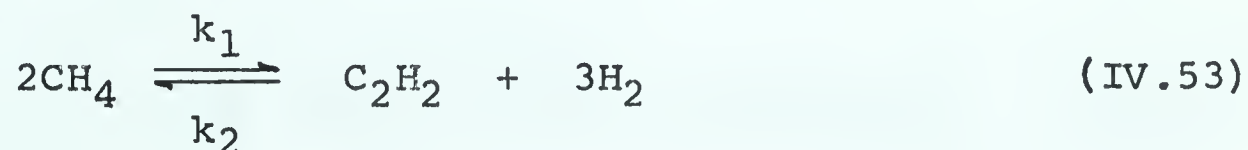
It can be seen from Table 7 that the close agreement with the implicit method suggests the calculational techniques, employed in the decoupling method, are free of gross errors and serve as a check on the soundness of the mathematical model.

IV.5.2 Example Problem No. 2

The decoupling method has been proved to be practicable and accurate, so that it may be applied to the design of a regenerative fixed-bed reactor. The problem, with design data taken from Kumagi et al(21), is stated as follows:

A regenerative refractory furnace is used to produce acetylene by the thermal cracking of methane. Pure methane at 950°K is fed at a rate of 20 lb-moles/(sq.ft.)(hr) into a pebble bed of alumina with radius 0.5 inches and a uniform initial temperature of 2000°K.

The main reaction is



where

$$k_1 = \exp (12.836 - 19214/T_g) \text{ sec}^{-1}$$

$$k_2 = \exp (4.358 - 5992/T_g) \text{ sec}^{-1} \quad (T_g \text{ } ^\circ\text{K})$$

$$\Delta H_{1400^\circ\text{C}} = 26,654 \text{ BTU/lb-mole CH}_4 \text{ converted}$$

The bed is 3 feet in length and has a porosity of 0.4. The convective heat transfer coefficient between the gas and the solid particles is estimated to be 46.1 BTU/(hr)(sq.ft.)(°R).

Other physical data are obtained from Perry's "Chemical Engineers' Handbook".

It is desired to find the temperature, fractional conversion and the pressure drop at various locations along the reactor as a function of time.

Accordingly the computational procedures follow those outlined in Case 4 of the previous problem, with the inclusion of reaction and pressure drop in the gas phase. Since the reaction is given to be reversible and 1st order, if ideal gas behavior is assumed, then the rate equation can be written as

$$R(x, P, T) = \frac{P}{R' T_g (1+x)} \left\{ k_1 (1-x) - k_2 x/2 \right\} \frac{\text{lb-mole}}{\text{sec.ft}^3} \quad (\text{IV.54})$$

The fractional conversion becomes

$$\begin{aligned} \frac{dx}{dz} = & \frac{P}{G_m^o R' T} \cdot \frac{3600}{(1+x)} \left\{ (1-x) \exp \left[(12.836 - 19.214/T_g) \right] \right. \\ & \left. - \frac{x}{2} \cdot \exp \left[(4.358 - 5.992/T_g) \right] \right\} \quad (\text{IV.55}) \end{aligned}$$

Similar to that for moving-bed reactor the energy balance in gas phase is

$$\begin{aligned} \frac{dT_g}{dz} = & \left\{ \frac{h_f a_s}{G_m^o} \cdot (T_s + q\Delta\theta/2 - T_g) - \left[(-C_{p1} + \frac{C_{p2}}{2} + \frac{3C_{p3}}{2}) \cdot \right. \right. \\ & \left. \left. (T_g - 1673) + 26,654 \right] \frac{dx}{dz} \right\} / \left[(1-x)C_{p1} + \frac{x}{2} C_{p2} + \frac{3x}{2} C_{p3} \right] \quad (\text{IV.56}) \end{aligned}$$

At 1000°C and 35% conversion, which represents the average values of the parameters, the viscosity of the gas is 0.03 cp. The density is given by

$$\begin{aligned}\rho_g &= \frac{16}{(1+x)(359)(T_g/273)(14.7/P)} \\ &= \frac{0.83 P}{(1+x) T_g} \quad (\text{IV.57})\end{aligned}$$

Upon substitution into equation (IV.4), the pressure drop becomes

$$\frac{dP}{dz} = \frac{(1+x) T_g}{P} \times 8.35 \times 10^{-4} \text{ (psi/ft)} \quad (\text{IV.58})$$

The results are all plotted in Graphs No. 6 and 7.

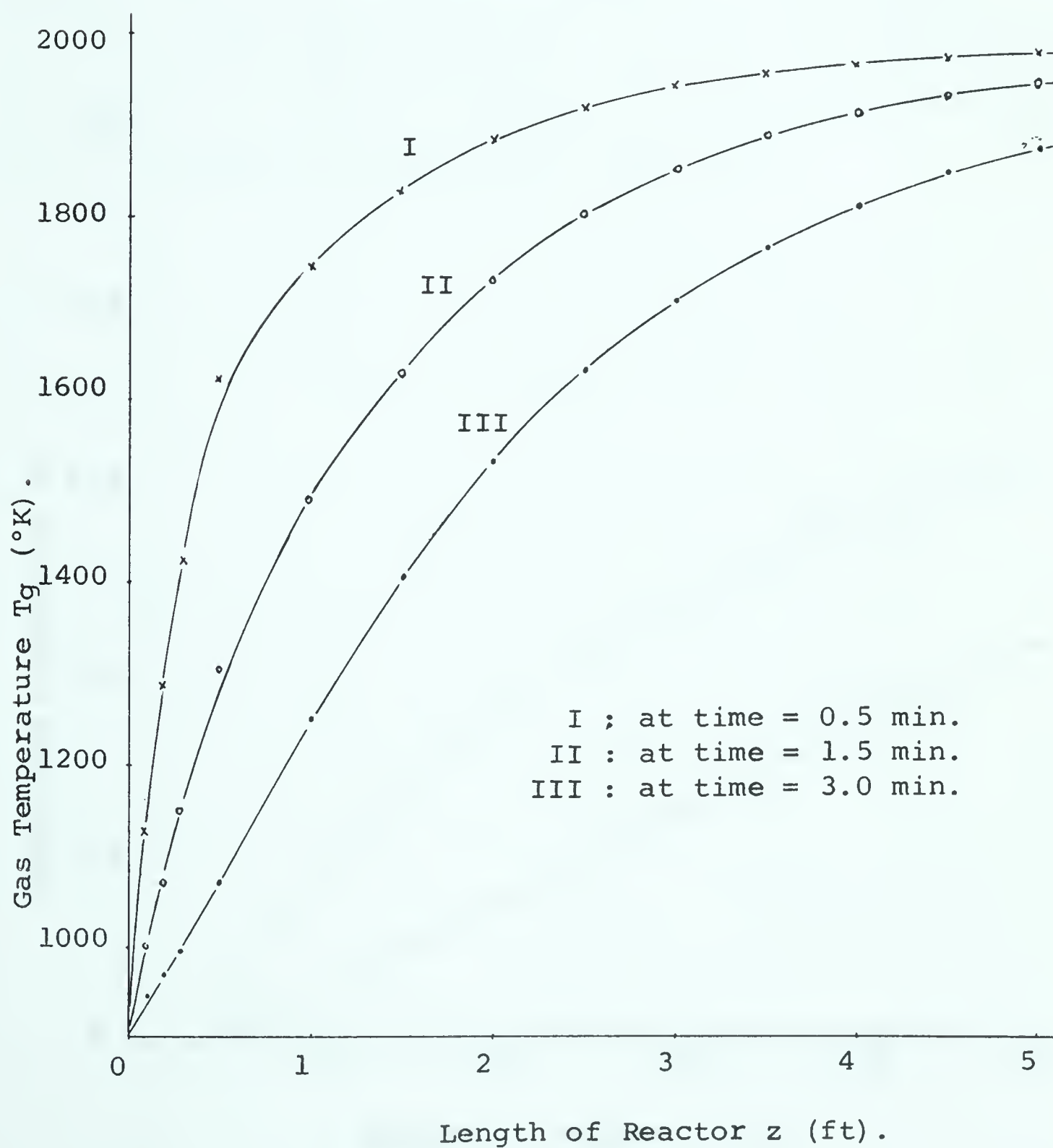
There is no experimental nor calculational check on these results, although the general trend appears reasonable.

IV.6 Summary

1. For fixed bed heat exchangers with no chemical reaction, the proposed implicit method which involves dividing the solid particles into a number of incremental shells and using a time average for the solid temperature and a position average for the gas temperature is a general and stable method that should be satisfactory.

Graph No. 6

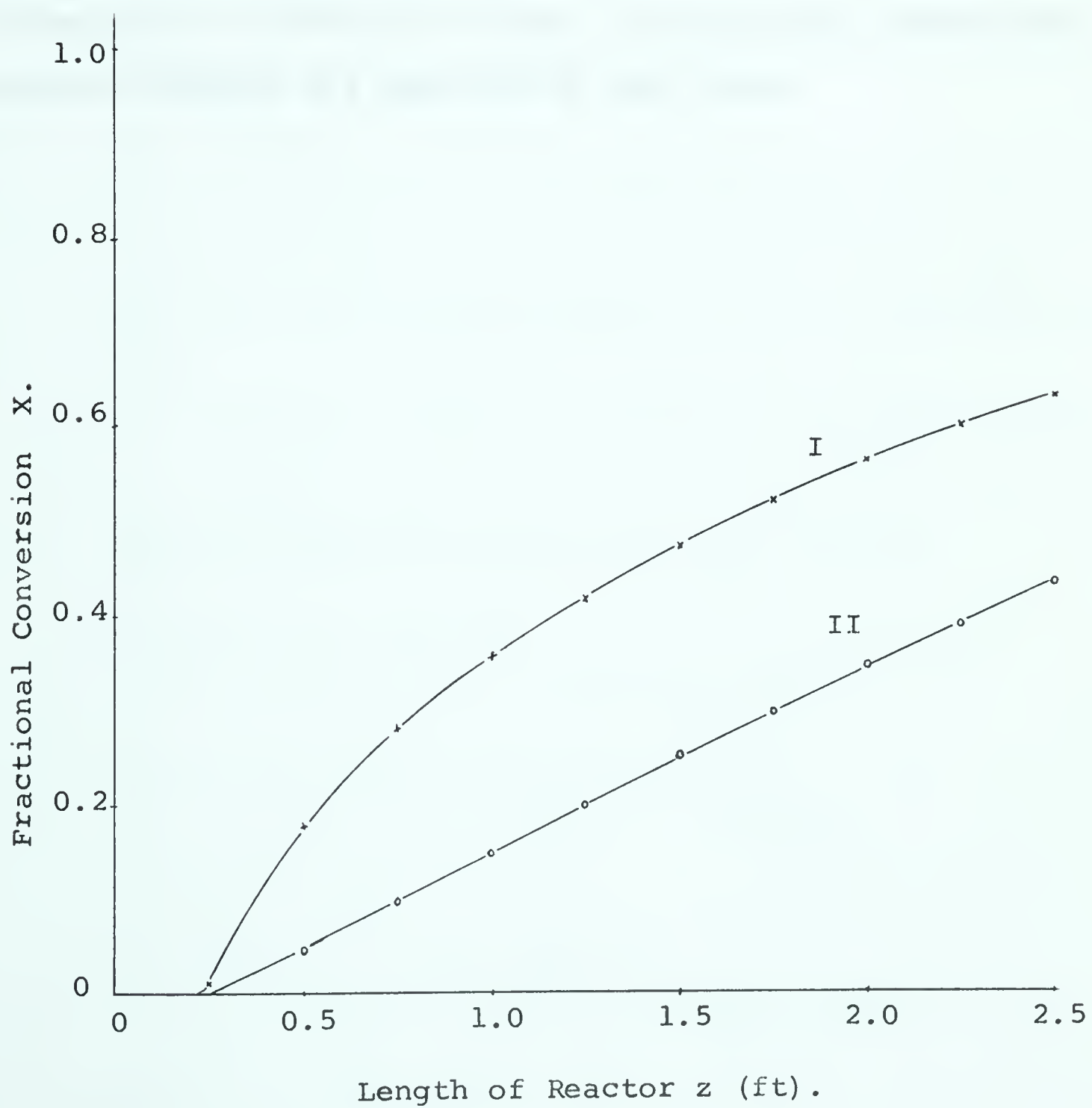
Gas Temperature Profile along the Fixed Bed Reactor
for the Production of Acetylene.



Graph No. 7

The Fractional Conversion of Methane along the
Fixed-bed Regenerative Reactor.

I : at time = 0.5 min.
II : at time = 3.0 min.



2. For fixed bed regenerative chemical reactors with reaction in the fluid phase only, the very large problem involving a system of non-linear partial differential equations can be reduced, by a decoupling technique into two much smaller problems involving, first, a linear partial differential equation and, second, a set of first order, non-linear, ordinary differential equations. An efficient computational technique for solving the former is presented; conventional explicit methods are employed on the latter.

NOMENCLATURE

A_s	Total surface area per unit volume of reactor space
C_a	Concentration of component a
C_{pm}	Molal heat capacity of gas
C_{pi}	Molal heat capacity of component i
c_f	Specific heat of gas
c_s	Specific heat of solid
D_p	Diameter of solid spheres
D_R	Inner diameter of reactor
G	Mass flow rate of gas per unit area cross-section
G_m	Molal flow rate of gas per unit cross-section area
G_s	Mass flow rate of solid spheres per unit cross-section area
h_f	Heat transfer coefficient between gas and solid spheres
h_w	Heat transfer coefficient between gas and reactor wall
ΔH_{T_b}	Heat of reaction at reference temperature T_b (positive for endothermic reaction)
k	Reaction rate constant
k_s	Thermal conductivity of solid spheres
K	Thermal diffusivity of solid spheres
P	Total pressure at any point z in reactor
Q_G	Enthalpy of gas
Q_s	Heat content of solid spheres
r	Radius variable from center of solid sphere
R	Radius of solid sphere
R'	Gas constant
$R(x, P, T_g)$	Rate of conversion of limiting reactant per unit volume of reactor

t	Time variable
T	Temperature variable of solid sphere
T_g	Temperature variable of gas
T_s	Surface temperature of solid sphere
T_w	Temperature of reactor wall
u_s	Velocity of solid spheres in moving bed
x	Fractional conversion of limiting reactant at point z in reactor
z	Distance variable along reactor from the entrance
ϵ	Fractional void in bed
ρ_g	Density of gas at point z in reactor
ρ_s	Density of solid spheres
θ	Reduced time variable defined in equation (IV.9)
μ	Viscosity of gas

Superscript

initial condition

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APPENDIX AFinite Difference ExpressionsWhich are Third Order Correct

If T_{n-2} , T_{n-1} , T_n , T_{n+1} are known and the spacings a , b , c are not necessarily equal, then by Taylor's expansion

$$T_{n+1} - T_n = a T'_n + \frac{a^2}{2} T''_n + \frac{a^3}{6} T'''_n$$

$$T_{n-1} - T_n = -b T'_n + \frac{b^2}{2} T''_n - \frac{b^3}{6} T'''_n$$

$$T_{n-2} - T_n = -c T'_n + \frac{c^2}{2} T''_n - \frac{c^3}{6} T'''_n$$

Hence,

$$T'_n = \frac{(T_{n+1} - T_n)c^2b^2(b-c) + (T_{n-1} - T_n)a^2c^2(c+a) - (T_{n-2} - T_n)a^2b^2(a+b)}{\Delta}$$

$$T''_n = \frac{(T_{n+1} - T_n)bc(b^2 - c^2) + (T_{n-1} - T_n)ac(a^2 - c^2) + (T_{n-2} - T_n)ab(b^2 - a^2)}{\Delta/2}$$

where

$$\Delta = abc \left\{ a(b^2 - c^2) - b(c^2 - a^2) - c(a^2 - b^2) \right\}$$

Differential Form	Finite Difference Expression	Geometrical Representation
$\frac{\partial T_n}{\partial r}$	$\frac{2T_{n+1} + 3T_n - 6T_{n-1} + T_{n-2}}{6 \Delta r}$	$\frac{T_{n-2} \quad T_{n-1} \quad T_n \quad T_{n+1}}{\cdot \quad \cdot \quad \cdot \quad \cdot}$
$\frac{\partial^2 T_n}{\partial r^2}$	$\frac{T_{n+1} - 2T_n + T_{n-1}}{\Delta r^2}$	
$\frac{\partial T_n}{\partial r}$	$\frac{32T_{n+\frac{1}{2}} - 15T_n - 20T_{n-1} + 3T_{n-2}}{30 \Delta r}$	$\frac{T_{n-2} \quad T_{n-1} \quad T_n \quad T_{n+\frac{1}{2}}}{\cdot \quad \cdot \quad \cdot \quad \cdot}$
$\frac{\partial^2 T_n}{\partial r^2}$	$\frac{16T_{n+\frac{1}{2}} - 25T_n + 10T_{n-1} - T_{n-2}}{5 \Delta r^2}$	
$\frac{\partial T_n}{\partial r}$	$\frac{11T_n - 18T_{n-1} + 9T_{n-2} - 2T_{n-3}}{12 \Delta r}$	$\frac{T_{n-3} \quad T_{n-2} \quad T_{n-1} \quad T_n}{\cdot \quad \cdot \quad \cdot \quad \cdot}$
$\frac{\partial^2 T_n}{\partial r^2}$	$\frac{2T_n - 5T_{n-1} + 4T_{n-2} - T_{n-3}}{\Delta r^2}$	
$\frac{\partial T_{n+\frac{1}{2}}}{\partial r}$	$\frac{184T_{n+\frac{1}{2}} - 225T_n + 50T_{n-1} - 9T_{n-2}}{60 \Delta r}$	$\frac{T_{n-2} \quad T_{n-1} \quad T_n \quad T_{n+\frac{1}{2}}}{\cdot \quad \cdot \quad \cdot \quad \cdot}$

APPENDIX BOutline of Runge-Kutta Method

$$\frac{dT_i}{dz} = T_i(z; T_1, \dots, T_i, \dots)$$

$$k_i' = \Delta z T_i(z; T_1, \dots, T_i, \dots)$$

$$k_i'' = \Delta z T_i\left(z + \frac{\Delta z}{2}; T_1 + \frac{k_1'}{2}, \dots, T_i + \frac{k_i'}{2}, \dots\right)$$

$$k_i''' = \Delta z T_i\left(z + \frac{\Delta z}{2}; T_1 + \frac{k_1''}{2}, \dots, T_i + \frac{k_i''}{2}, \dots\right)$$

$$k_i^{iv} = \Delta z T_i(z + \Delta z; T_1 + k_1''', \dots, T_i + k_i''', \dots)$$

Therefore,

$$\Delta T_i = \frac{1}{6} \left\{ k_i' + 2(k_i'' + k_i''') + k_i^{iv} \right\}$$

All the k_i' are evaluated before the k_i'' are calculated, similarly the k_i''' and k_i^{iv} are evaluated sequentially. If Runge-Kutta-Gill is used the coefficients will be different but they are given in reference (8).

APPENDIX CStability of the Diffusion Equation

Consider an I.V.P. of heat conduction

$$\frac{\partial u}{\partial \theta} = K \frac{\partial^2 u}{\partial x^2} \quad 0 < x < L \quad (1)$$

with

$$\begin{aligned} u(x, 0) &= \varphi(x) \\ u(0, \theta) &= 0 \\ u(L, \theta) &= 0 \end{aligned} \quad (2)$$

If $u(x, \theta)$ is the exact solution and $u_{j,n}$ is the finite difference solution then

$$u(x, \theta) = \sum_{n=1}^{\infty} A_n \sin \frac{n\pi x}{L} \exp \left(-K \left(\frac{n\pi}{L} \right)^2 \theta \right) \quad (3)$$

where A_n is obtained from expanding $\varphi(x)$ into an infinite orthogonal series such that

$$A_n = \frac{2}{L} \int_0^L \varphi(x) \cdot \sin \left(\frac{n\pi}{L} \cdot x \right) dx$$

Expressing (1) in finite difference forms of

(i) explicit, forward difference

$$u_{j,n+1} = u_{j,n} + \beta (u_{j-1,n} - 2u_{j,n} + u_{j+1,n}) \quad (4)$$

(ii) implicit, backward difference

$$\begin{aligned}
 -u_{j-1,n+1} + \left(2 - \frac{1}{\beta}\right) u_{j,n+1} - u_{j+1,n+1} \\
 = u_{j,n} \frac{1}{\beta}
 \end{aligned} \tag{5}$$

(iii) implicit, Crank-Nicholson method

$$\begin{aligned}
 -u_{j+1,n+1} + 2\left(1 + \frac{1}{\beta}\right) u_{j,n+1} - u_{j+1,n+1} \\
 = u_{j-1,n} - 2\left(1 - \frac{1}{\beta}\right) u_{j,n} + u_{j+1,n}
 \end{aligned} \tag{6}$$

where

$$\beta = \Delta\theta/\Delta x^2$$

Now define the error as

$$\epsilon_{j,n} = u_{j,n} - u(j\Delta x, j\Delta\theta)$$

and substituting into (4) it gives

$$\epsilon_{j,n+1} = \beta \epsilon_{j+1,n} + (1 - 2\beta) \epsilon_{j,n} + \beta \epsilon_{j-1,n} \tag{7}$$

By separation of variable, solution of equation (7) may be written as

$$\epsilon_{j,n} = f(e^{\alpha j\Delta\theta}, e^{i\gamma n\Delta x}) \tag{8}$$

Substituting into (7) and simplifying gives

$$\begin{aligned} e^{\alpha\Delta\theta} &= \beta e^{i\gamma\Delta x} + (1 - 2\beta) + \beta e^{-i\gamma\Delta x} \\ &= 1 - 4\beta \sin^2 \left(\frac{\gamma\Delta x}{2} \right) \end{aligned} \quad (9)$$

In order that the error $\epsilon_{j,n}$ at any fixed point, $n\Delta x$, will not grow as θ increases, it is necessary and sufficient that

$$\left| e^{\alpha\Delta\theta} \right| \leq 1$$

i.e.

$$-2 \leq -4\beta \sin^2 \left(\frac{\gamma\Delta x}{2} \right) \leq 0$$

or

$$\beta \leq \frac{1}{2} \quad (10)$$

By this procedure one can establish the stability ratio of the above finite difference forms:

(i) explicit

$$\left| e^{\alpha\Delta\theta} \right| \leq 1 - 4\beta \sin^2 \left(\frac{\gamma\Delta x}{2} \right) \leq 1 \quad (11)$$

(ii) backward difference

$$\left| e^{\alpha\Delta\theta} \right| \leq 1 / \left(1 + 4\beta \sin^2 \frac{\gamma\Delta x}{2} \right) \leq 1 \quad (12)$$

(iii) Crank-Nicholson form

$$\left| e^{\alpha\Delta\theta} \right| \leq \left\{ 2 - 4\beta \sin^2 \left(\frac{\gamma\Delta x}{2} \right) \right\} / \left(1 + 4\beta \sin^2 \frac{\gamma\Delta x}{2} \right) \leq 1 \quad (13)$$

Thus, (ii) and (iii) are unconditionally stable.

APPENDIX D

Verification of Equation (IV.43) in
Satisfying the Initial Condition

Since Equation (IV.43) is the sum of equations (IV.31) and (IV.42), at $\theta=0$ equation (IV.31) is zero; it is necessary, therefore to prove that equation (IV.42) does satisfy the initial condition $T(r)$.

Lemma:

If $f(x)$ is an even function of x , which can be expanded, so will be $f(x \pm 2nR)$, in a Fourier series of cosines of multiples of $\pi x/R$, then

$$\sum_{n=-\infty}^{\infty} f(x+2nR) = \frac{1}{R} \int_0^{\infty} f(x) dx$$

$$+ \frac{2}{R} \sum_{n=1}^{\infty} \cos \frac{n\pi x}{R} \int_0^{\infty} f(x') \cos \frac{n\pi x'}{R} dx' \quad (i)$$

provided the integrals are convergent and the series will converge.

Proof of the lemma can be referred in any standard text on Fourier Transforms.

Now let $f(x) = e^{-x^2/4K\theta}$, then

$$\begin{aligned}
& \sum_{n=-\infty}^{\infty} \exp \left(- \frac{(x + 2nR)^2}{4K\theta} \right) = \frac{1}{R} \int_0^{\infty} \exp \left(- \frac{x^2}{4K\theta} \right) dx \\
& + \frac{2}{R} \sum_{n=1}^{\infty} \cos \frac{n\pi x}{R} \int_0^{\infty} \exp \left(- \frac{x'^2}{4K\theta} \right) \cos \frac{n\pi x'}{R} dx' \\
& = \frac{\sqrt{\pi K\theta}}{R} \left\{ 1 + 2 \sum_{n=1}^{\infty} \cos \frac{n\pi x}{R} \exp \left(- \frac{Kn^2\pi^2\theta}{R^2} \right) \right\} \quad (ii)
\end{aligned}$$

Here letting $\eta = x/2\sqrt{K\theta}$ and $b = n\pi\sqrt{K\theta}/R$

$$\int_0^{\infty} \exp \left(- \frac{x^2}{4K\theta} \right) \cos \frac{n\pi x}{R} dx = 2\sqrt{K\theta} \int_0^{\infty} e^{-\eta^2} \cos (2b\eta) d\eta \quad (iii)$$

From the contour integral

$$\int_c e^{-z^2} dz = 0 \quad \text{for } z = \eta + i\xi \quad (iv)$$

where c is the contour of the rectangle $-a \leq \eta \leq a$, $0 \leq \xi \leq b$ and taking the limit of a approaches infinity it yields

$$\int_0^{\infty} e^{-\eta^2} \cos (2b\eta) d\eta = 1/2 \cdot \sqrt{\pi} \exp (-b^2) \quad (v)$$

Hence, the equation (ii)

Replacing x by $(r' - r)$ and $(r + r)$, equation (IV.42) yields upon simplification

$$u = \frac{2}{rR} \int_0^R T(r') r' \sum_{n=1}^{\infty} \exp\left(-\frac{Kn^2 \pi^2 \theta}{R^2}\right) \sin \frac{n\pi r}{R} \sin \frac{n\pi r'}{R} dr' \quad (\text{vi})$$

which is equation (IV.32).

at $\theta = 0$

$$u_0 = \frac{1}{R} \sum_{n=1}^{\infty} \frac{\sin \frac{n\pi r}{R}}{r/2} \int_0^R r' T(r') \sin \frac{n\pi r'}{R} dr' \quad (\text{vii})$$

Now assuming that $rT(r)$ can be expressed into an infinite orthogonal series of $\sin \frac{n\pi r}{R}$

i.e.

$$rT(r) = \sum_{n=1}^{\infty} B_n \cdot \sin \frac{n\pi r}{R}$$

then

$$B_n = \frac{\int_0^R r' T(r') \cdot \sin\left(\frac{n\pi}{R} r'\right) \cdot dr'}{\int_0^R \sin^2\left(\frac{n\pi}{R} r'\right) dr'}$$

$$= \frac{\int_0^R r' T(r') \sin\left(\frac{n\pi}{R} r'\right) dr'}{R/2} \quad (\text{viii})$$

Therefore,

$$rT(r) = \sum_{n=1}^{\infty} \frac{\sin\left(\frac{n\pi}{R} r\right)}{R/2} \int_0^R r' T(r') \sin\left(\frac{n\pi}{R} r'\right) dr' \quad (\text{ix})$$

so

$$u_0 = T(r) \quad \text{Q.E.D.}$$

APPENDIX ENumerical Evaluation of Error Cofunction

By definition

$$\operatorname{erfc}(x) = 1 - \operatorname{erf}(x)$$

and

$$\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt$$

From mathematical tables values of $\operatorname{erf}(x_i)$ are read into the memory of the digital computer. To evaluate $\operatorname{erfc}(x_j)$ where $x_i < x_j < x_{i+1}$, let

$$\Delta x = \frac{x_j - x_i}{6}$$

and

$$y_k = \exp(-(x_i + k\Delta x)^2)$$

$$\text{for } k = 0, 1, \dots, 6$$

Then by Newton's forward formula of integration for the 6th degree

$$\begin{aligned} \operatorname{erfc}(x_j) = 1 - \operatorname{erf}(x_i) - \frac{2\Delta x}{140\sqrt{\pi}} \\ \cdot (41y_0 + 216y_1 + 27y_2 + 272y_3 \\ + 27y_4 + 216y_5 + 41y_6) \end{aligned}$$

APPENDIX FListings of Computer Programs andSample Outputs

1. Moving Bed Heat Exchanger Design
2. Moving Bed Reactor Design
3. Regenerative Bed Heat Exchanger - Analytical
4. Regenerative Bed Heat Exchanger - Implicit
5. Regenerative Bed Heat Exchanger - Decoupling
6. Acetylene Production in Regenerative Bed - Decoupling


```

$JOB          140034 MOVING BED HEAT EXCHANGER.
$TIME         5.510
$IRJOB MOVING GO
$HEATC HEAT  NODECK, VOL (RT

```

```

C DESIGN OF MOVING BED HEAT EXCHANGER BY PAPER LINE THE DIFFERENTIAL
C EQUATION INTO A SET OF TWO FIRST ORDER O.D.E., TOGETHER WITH THE
C GAS EQUATION ARE SOLVED BY RUNGE-KUTTA-ILL METHOD.
C ALL INPUT DATA ARE IN LB, HP, FT, DEG F, UNITS.
C MAXIMUM NO. OF DIVISIONS IN RANGE OF SOLID IS 20.
C IF NECESSARY, CHANGE THE FORMAT OF INPUT AND OUTPUT.

```

```

C GS, GA - MASS FLOW RATE OF SOLID AND GAS RESPECTIVELY.
C CS, CP - SPECIFIC HEAT OF SOLID AND GAS RESPECTIVELY.
C TO, TGO - INITIAL TEMPERATURES OF SOLID AND GAS RESPECTIVELY.
C DS - DENSITY OF SOLID SPHERE.
C R - RADIUS OF SOLID SPHERE IN INCH.
C SK - THERMAL CONDUCTIVITY OF SOLID SPHERE.
C VD - FRACTIONAL VOID OF THE MOVING BED.
C HE - HEAT TRANSFER COEFFICIENT BETWEEN GAS AND SOLID SPHERE.
C DL - INCREMENT OF EXCHANGER LENGTH IN FEET.
C M - NO. OF DIVISIONS ALONG THE MOVING CARRIER.
C TS - TEMPERATURE AT THE SURFACE OF SOLID SPHERE.
C RTS - NORMALIZED SURFACE TEMPERATURE (TS-TO)/(TGO-TO).
C TG - GAS TEMPERATURE VARIABLE.
C PTG - NORMALIZED GAS TEMPERATURE (TG-TO)/(TGO-TO).

```

```

C OUTPUT DATA ARE IN SET OF THREE LINES --
C DISTANCE IN FEET AND REDUCED DISTANCE OF THIRD (1/3) OF
C TS, RTS, TG AND PTG
C SOLID TEMPERATURES AT ALTERNATING SPHERICAL CELL FROM CENTER.

```

```

DIMENSION F(20), GA(20), GR(20), DC(20), DD(20), S(20), R(20)

```

```

READ (5,1) GS, CS, DS, SK, R, VD

```

```

1 FORMAT (F8.2, F6.2, F7.2, F7.2, F7.2, F7.2)

```

```

READ (5,2) GA, CP, HE, DL, M, TO, TGO

```

```

2 FORMAT (F8.2, F6.2, F7.2, F6.2, 2X, 12, F7.2, F7.2)

```

```

MA=M+1

```

```

MB=M-1

```

```

FM=M

```

```

R=R/12.0

```

```

H=R/FM

```

```

TH=SK/(CS*DS)

```

```

US=GS/(DS*(1.0-VD))

```

```

AD=TH/(H*H*US)

```

```

PED=TH/(DS*D*R)

```

```

RA=3.0*HE*(1.0-VD)/(GA*CP*R)

```

```

S1=12.0*FM-12.0

```

```

S2=120.0*FM-140.0

```



```

      F3=300.0*FM-70.0
      F4=100.0*FM+30.0
      F5=20.0*(2.0*F4-1.0)
      XA=SQRT(2.0)
      PA=(XA-1.0)/2.0
      PR=(2.0-XA)/2.0
      PC=-XA/2.0
      PD=(2.0+XA)/2.0
      PT=60.0*HF*H/SK
      RTT=104.0+4*PT
      DTSI=0.00
      DO 3 I=1,M
3      T(I)=T0
      T(MA)=TGO
101    DO 10 I=1,MA
10      Y(I)=T(I)
      CR=1.0
100    F(1)=AP*(-26.0*Y(1)+25.0*Y(2)-Y(3))/K.0
      F(2)=AP*(-Y(1)-12.0*Y(2)+13.0*Y(3))/K.0
      DO 11 J=3,MP
      FJ=J
      FA=2.0*Y(J-2)/(6.0*FJ-7.0)+(2.0*FJ-5.0)*Y(J-1)/(2.0*FJ-7.0)
      FH=-4.0*(FJ-1.0)*Y(J)/(2.0*FJ-1.0)+(6.0*FJ+1.0)*Y(J+1)/(6.0*FJ-9.0)
11      F(J)=AP*(FA+FH)
      FS=(R1*Y(MA)+225.0*Y(1)-50.0*Y(2-1)+5.0*Y(3-2))/RTT
      F(M)=AP*(-21*Y(0-2)+-2*Y(1-1)-13*Y(1)+34*Y(1))/RTT
      F(MA)=RAX*(Y(MA)-T5)
      IF (CR.GT.1.0) GO TO 13
      DO 12 I=1,MA
      QA(I)=F(I)*DL
12      Y(I)=T(I)+QA(I)/2.0
      CR=CR+1.0
      GO TO 100
13      IF (CR.GT.2.0) GO TO 15
      DO 14 I=1,MA
      QB(I)=F(I)*DL
14      Y(I)=T(I)+QA(I)*PA+QB(I)*PR
      CR=CR+1.0
      GO TO 100
15      IF (CR.GT.3.0) GO TO 17
      DO 16 I=1,MA
      QC(I)=F(I)*DL
16      Y(I)=T(I)+QB(I)*PC+QC(I)*PD
      CR=CR+1.0
      GO TO 100
17      DO 18 I=1,MA
      QD(I)=F(I)*DL
18      T(I)=T(I)+(QA(I)+QB(I))/6.0+(PR*QB(I)+PD*QC(I))/K.0
      FS=(R1*Y(MA)+225.0*Y(1)-50.0*Y(2-1)+5.0*Y(3-2))/RTT

```



```

RTS=(TS-T0)/(T50-T0)
RTG=(T(MA)-T0)/(T(M)-T0)
DIST=D(SI+DL)
REFDIST=REFD*DIST
WRITE (6,5) DIST, REFDIST
5  FORMAT (1H0, 2X, (1HDISTAX = , F7.2, 4H 51., 2X, (1HREFDISTAX = , F7.2, 4H 51., 2X, 14HEND OF L
1H, 2X, F13.6)
WRITE (6,6) TH, RTS, T(9A), T10
6  FORMAT (1H , 2X, REFS = , F7.2, 4H 08, F14.6, 3X, RHTF = , F7.2,
14H 08, F15.6)
WRITE (6,7) (T(I), I=1,10,2)
7  FORMAT (1H , 5X, 6F11.2)
IF (RTG.LT.2.5) GO TO 101
WRITE (6,8)
8  FORMAT (1H-, 15X, 20HEND OF CALCULATION. )
END

$ENTRY HEAT
2232.00 0.280 162.00 1.300 1.000 0.50
2500.00 0.250 78.00 0.020 100.00 200.00

```


(SAMPLE 100(PH))

FIGURE 3. MOVING-HEAD HEAT EXCHANGER DESIGN.

DISTANCE = 0.100 FT.	REDUCED LENGTH = 0.14124E+01
TS = 184.01 OR 0.846147E+01	TG = 217.77 OR 0.117002E+01
100.00 100.01 100.17 100.77 107.78	
DISTANCE = 0.200 FT.	REDUCED LENGTH = 0.28240E+01
TS = 172.17 OR 0.731742E+01	TG = 220.31 OR 0.127312E+01
100.10 100.39 102.21 10.91 106.77	
DISTANCE = 0.300 FT.	REDUCED LENGTH = 0.443712E+01
TS = 187.43 OR 0.874318E+01	TG = 241.81 OR 0.141806E+01
100.96 102.19 107.12 121.20 101.71	
DISTANCE = 0.400 FT.	REDUCED LENGTH = 0.607616E+01
TS = 201.04 OR 0.101041E+01	TG = 213.83 OR 0.133823E+01
103.48 106.05 114.20 132.72 168.63	
DISTANCE = 0.500 FT.	REDUCED LENGTH = 0.742520E+01
TS = 213.77 OR 0.113767E+01	TG = 260.77 OR 0.160067E+01
108.02 111.87 122.13 148.17 178.81	
DISTANCE = 0.600 FT.	REDUCED LENGTH = 0.879423E+01
TS = 225.96 OR 0.125964E+01	TG = 277.12 OR 0.177123E+01
114.39 118.57 132.15 150.17 170.16	
DISTANCE = 0.700 FT.	REDUCED LENGTH = 0.104730E+02
TS = 237.83 OR 0.114829E+01	TG = 283.67 OR 0.185167E+01
122.19 123.89 142.10 166.79 192.76	
DISTANCE = 0.800 FT.	REDUCED LENGTH = 0.113023E+02
TS = 249.48 OR 0.143477E+01	TG = 299.93 OR 0.199930E+01
131.04 137.20 152.60 178.11 214.70	
DISTANCE = 0.900 FT.	REDUCED LENGTH = 0.134714E+02
TS = 260.98 OR 0.160980E+01	TG = 371.24 OR 0.212241E+01
140.64 147.27 167.28 189.41 226.76	
DISTANCE = 1.000 FT.	REDUCED LENGTH = 0.149014E+02
TS = 272.39 OR 0.172387E+01	TG = 327.52 OR 0.227152E+01
150.75 157.67 174.12 200.68 238.78	
DISTANCE = 1.100 FT.	REDUCED LENGTH = 0.164094E+02
TS = 283.73 OR 0.184122E+01	TG = 333.77 OR 0.237788E+01
161.22 168.22 185.70 211.33 249.78	
DISTANCE = 1.200 FT.	REDUCED LENGTH = 0.180871E+02
TS = 301.79 OR 0.201786E+01	TG = 331.75 OR 0.251715E+01
178.43 185.73 202.90 229.31 267.17	

END OF CALCULATION.


```

SUON      150001  MOVING BED REACTOR DESIGN.
TIME      5,000
MOVING    50
DIRECT REACT  NO LIST, NITROX

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```

C  A SPECIFIC PROGRAM DEVELOPED TO VIEW OF THE MOVING BED HEAT
C  EXCHANGER FOR THERMAL CONVERSION OF HYDROGEN.
C  ALL INPUT DATA ARE IN IN, HM, FT, MU, DEG F, MMHG SPECIFIC.
C  THE RADIUS OF SOLID SPHERE HAS BEEN DIVIDED INTO 5 EQUAL SPHERES.
C
C  DZ - INCREMENT OF REACTOR LENGTH IN FEET.
C  SK - THERMAL CONDUCTIVITY OF SOLID SPHERES.
C  SC - SPECIFIC HEAT OF SOLID SPHERES.
C  SD - DENSITY OF SOLID SPHERES.
C  SU - VELOCITY OF THE MOVING BED.
C  SR - RADIUS OF SOLID SPHERE.
C  HF - HEAT TRANSFER COEFFICIENT BETWEEN GAS AND SOLID SPHERES.
C  SA - SURFACE AREA OF SOLID PER UNIT VOLUME OF BED.
C  GMD - INITIAL MOLAR FLOW RATE OF GAS.
C  CP4, CP5, CP6 - MOLAR SPECIFIC HEAT OF METHANE, ETHYLENE AND
C  HYDROGEN RESPECTIVELY.
C  VQ - VOID FRACTION OF MOVING BED.
C  TS - SOME REFERENCE TEMPERATURE.
C  DH1 - HEAT OF REACTION AT REFERENCE TEMPERATURE.
C  GR - UNIVERSAL GAS CONSTANT (1545.06 FT.LB/MOLE.DEG.F.).
C  FRAC1 - FRACTIONAL CONVERSION OF REACTANT IN 1ST REACTOR.
C  IG - GAS TEMPERATURE VARIABLE.
C  X - FRACTIONAL CONVERSION VARIABLE.
C  P - TOTAL PRESSURE VARIABLE IN REACTOR (PSIA).
C  L - LENGTH OF REACTOR FROM BED INLET.
C  ST - SURFACE TEMPERATURE OF SOLID SPHERES AT 1.

```

```

C  DIMENSION F(10), P(10), Q(10), R(10), S(10), T(10), U(10)
100 READ (5,7) DZ
7  FORMAT (F5.2)
IF (DZ.(E3.0)) GO TO 101
READ (5,1) SK, SC, SD, SU, SR
1  FORMAT (F6.2, F8.4, F6.2, F8.2, F6.4)
READ (5,2) HF, SA, GMD, CP4, CP5, CP6
2  FORMAT (F5.2, F8.2, F7.2, F6.2)
READ (5,3) VQ, GR, DH1, SR, FRAC1
3  FORMAT (F5.2, F7.1, F6.1, F6.1, F7.3)
WRITE (6,2) DZ
4  FORMAT (1H-, 5X, 20HINITIAL INCREMENT = , F6.2)
WRITE (6,14)
14  FORMAT (1H-, 8X, 2HIG, 8X, 2H1Z, 8X, 2H1S, 8X, 2H14, 8X, 2H17, 8X,
2H1T )
WRITE (6,15)
15  FORMAT (1H-, 14X, 2HIG, 16X, 14X, 14X, 14X, 14X, 14X )
C  CALCULATION OF VARIOUS CONSTANTS.
H=SR/60.0

```


AP=SK/(SC*SI*SI*H*H)

HT=60.0*H*H/HK

GA=992.0/(194.0+HT)

FA=0.0*(GA-42.0)

FR=-50.0*(GA+42.0)

FC=225.0*(GA-141.0)

FD=GA*HT

CA=FR*FA/GM0

CPM=-CPA+2.0*CPB+CPD

CP=1.0/(GM0*GR)

XA=SQRT(2.0)

UA=(XA-1.0)/2.0

UB=(2.0-XA)/2.0

UC=-XA/2.0

UD=(2.0+XA)/2.0

DL=0.0

INPUT OF INITIAL DATA.

READ (5,4) (Y(I), I=1,8)

FORMAT (F0.3)

COUNT=1.0

IF (COUNT.GT.10.0) GO TO 14

Z=DZ

GO TO 18

IF (COUNT.GT.20.0) GO TO 17

Z=DZ+DZ

GO TO 18

Z=3.0*DZ

DO 19 J=1,8

T(I)=Y(I)

PC=1.0

SOLUTION OF PROBLEM BY RUNGE-KUTTA-FILL METHOD.

F(1)=AP*(-26.0*T(1)+27.0*T(2)-T(3))/4.0

F(2)=AP*(-T(1)-12.0*T(2)+13.0*T(3))/4.0

F(3)=AP*(2.0*T(1)+3.0*T(2)-24.0*T(3)+19.0*T(4))/17.0

F(4)=AP*(2.0*T(2)+9.0*T(3)-30.0*T(4)+21.0*T(5))/21.0

TS=(9.0*T(3)-11.0*T(4)+22.0*T(5)+10*T(6))/(1.4+HT)

TK=(12.45-22100.0/T(6))/0.434294

TR=3600.0*EXP(TK)

F(5)=AP*(992.0*TS-141.0*T(5)+42.0*T(4)-42.0*T(3))/20.0

F(7)=CR*T(8)*(1.0-T(7))*TR/(T(6)*(1.0+2.0*T(7)))

FA=((T(6)-TR)*CA+DH)*F(5)

F(6)=(CA*(TS-T(6))-FA)/(CP+T(7)*F(5))

F(8)=-0.01*(7.0+2.0*T(7))*T(6)/T(7)

IF (PC.GT.1.0) GO TO 22

DO 22 J=1,8

P(I)=2*F(I)

T(I)=Y(I)+P(I)/2.0

PC=PC+1.0

GO TO 20

IF (PC.GT.2.0) GO TO 26

DO 26 J=1,8

$$r_1 = r_1 + 1.0$$
$$Q(1) = \angle * \vdash (1)$$

25 $f(1) = \gamma(1) + 10 \times 2(1) + (1 \times 2)(1)$

750 100 200

26. If $(-1, 4, 0)$ is a point on the line

$$111) \quad \gamma \gamma \rightarrow \pi^0 \pi^0, \pi^0 \eta$$
$$T(1) = 2 \times (1)$$
$$Z_C \quad \tilde{f}(1) = f(1) + (1) * (1) + (1) * (1) + (1) * (1)$$
$$R(\cdot) = R(\cdot + 1) \cdot \psi$$

(5) 10 20

$$30 \quad 100 \quad 51 \quad 1 = 1, 2$$
$$\angle(1) = \angle \star + \angle(1)$$
$$x(t) = y(t) + (p(t) + q(t)) / r + (p^*(t) + q^*(t)) / r^* + \dots$$
$$111 = 11 + 2$$

END OF ONE INTERVAL MODULATION.

$$f_1 = (1) \cdot 1 + (-1) \cdot 2 + (-1) \cdot 3 + (-1) \cdot 4 + (-1) \cdot 5 + (-1) \cdot 6 + (-1) \cdot 7 + (-1) \cdot 8 + (-1) \cdot 9 + (-1) \cdot 10 = -40$$
$$W(R) = (5, 5) \quad Y(1), \quad Y(2), \quad Y(3), \quad Y(4), \quad Y(5) = 1$$

FORMAT (1H, 2X, 5F11.4)

$$W \in \mathcal{L}(\mathbb{R}^n, \mathbb{R}^n) \quad (b, b) = 1(b), \quad Y(b) = 1(b), \quad Y(b) = 1(b), \quad Y(b) = 1(b)$$

6. FORMAT (1H, 10A, F10.1, 10A, 10.4, 10A, 1. , 10A, F(.))

IF (117)•GE•FREE) 150 10 33

$$\text{COUNT} = \text{COUNT} + 1 \bullet$$

60 10 11

34 WRIT (6, 2)

50 10 1 10

THE FINDINGS

(ND)

SINIRI RAO

١٠١

1. 100 0.2500 100.00 522.10 0.00 1.00

21.60 725.10 42.60 47.30 21.00 5.10

5.4' 1000' 1-100' 5.7' 5.8'

246 • UUU

240. • 92

245 • 1111

145 • 100

146

5.60. 1963

1) $\alpha \in \mathbb{R}$,

34. 5.

1

(SAMPLE OUTPUT)

194001 000100 0000 0000 0000 0000.

INITIAL INCREMENT = 0.000

11	12	13	14	15	16
IG		A			L
2400.001	2400.001	2400.001	2400.001	2400.001	2400.001
1540.484		0.0000	34.000		0.000
2459.984	2459.984	2459.984	2459.984	2459.984	2459.984
1114.587		0.0000	34.000		0.000
2459.874	2459.874	2459.874	2459.874	2459.874	2459.874
1182.345		0.0000	34.000		0.000
2459.551	2459.551	2459.551	2459.551	2459.551	2459.551
1240.459		0.0000	34.000		0.000
2458.801	2458.801	2458.801	2458.801	2458.801	2458.801
1500.321		0.0000	34.000		0.000
2457.640	2457.640	2457.640	2457.640	2457.640	2457.640
1360.073		0.0000	34.000		0.000
2455.772	2455.772	2455.772	2455.772	2455.772	2455.772
1411.059		0.0000	34.000		0.000
2453.174	2453.174	2453.174	2453.174	2453.174	2453.174
1452.334		0.0000	34.000		0.000
2449.822	2449.822	2449.822	2449.822	2449.822	2449.822
1502.061		0.0000	34.000		0.000
2445.704	2445.704	2445.704	2445.704	2445.704	2445.704
1544.400		0.0000	34.000		0.000
2435.344	2435.344	2435.344	2435.344	2435.344	2435.344
1614.223		0.0000	34.000		0.000
2370.711	2370.711	2370.711	2370.711	2370.711	2370.711
1822.229		0.0000	34.000		0.000
2174.361	2174.361	2174.361	2174.361	2174.361	2174.361
1911.439		0.2352	34.637		0.000
2044.086	2044.086	2044.086	2044.086	2044.086	2044.086
1912.907		0.4941	34.043		1.200
1977.737	1977.737	1977.737	1977.737	1977.737	1977.737
1904.563		0.6220	33.011		1.000
1939.414	1939.414	1939.414	1939.414	1939.414	1939.414
1894.385		0.7008	32.812		2.400
1916.204	1916.204	1916.204	1916.204	1916.204	1916.204
1886.166		0.7521	31.644		0.000
1900.097	1900.097	1900.097	1900.097	1900.097	1900.097
1878.671		0.7583	30.728		3.600
1888.467	1888.467	1888.467	1888.467	1888.467	1888.467
1872.414		0.6152	29.754		4.200
1870.671	1870.671	1870.671	1870.671	1870.671	1870.671
1867.216		0.4359	28.736		0.000
1873.726	1873.726	1873.726	1873.726	1873.726	1873.726
1863.446		0.0000	27.833		0.000

END OF RUN COMPLETE (SAMPLE OUTPUT).

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2639		2640	
2641		2642	
2643		2644	
2645		2646	
2647		2648	
2649		2650	
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2761		2762	
2763		2764	
2765		2766	
2767		2768	
2769		2770	


```

      IF (1.0001.5).T(L+1).ND 1) GO TO 30
20  J=J+1
21  JL=J+L
      A=ZA*A(J)/(A(J)+A(JL))
      T(L+1)=T(L+1)+A
      IF (1A.GF.0.0001) GO TO 23
22  L=L+1
      GO TO 19
23  J=J+1
      GO TO 21
30  M=M+1
      TGR=0.00
      DO 31 I=1,M
31  TGR=TGR+T(I)
      TGR=TGR/EXP(T(N)+Z)
      TEMP=TSO+DTEMP*TGR
      WRITE (6,3) T(N), TGR, TEMP
3  FORMAT (1H, 15X, F8.4, 3X, F7.1, 3X, F7.3)
      IF (N.GF.NA) GO TO 33
32  N=N+1
      GO TO 100
33  CONTINUE
      GO TO 50
32  CONTINUE
      END

```

```

$PRINT ANALY F
13 280.10 70.00
0.10416667E+00
0.02083333E+00
0.03333333E+00
0.10416667E+01
0.15625000E+01
0.20833333E+01
0.00

```


(CONTINUED OUTPUT)

TABLE 1. DEGENERATIVE SCORING OF EXHIBITS - ANALYTICAL.

AT 0.833333E+00 MTN.

0.6151	0.76723	373.710
1.2303	0.56896	313.710
1.8454	0.41030	313.727
2.4605	0.29017	307.312
3.0757	0.18177	284.124
3.6908	0.13433	280.635
4.3059	0.09277	286.863
4.9210	0.06289	284.402
5.5362	0.04181	282.726
6.1513	0.02757	281.936
6.7664	0.01806	281.284
7.3816	0.01173	280.823
7.9967	0.00761	280.532

AT 0.208333E+01 MTN.

0.6151	0.91849	344.274
1.2303	0.81863	336.604
1.8454	0.68781	328.147
2.4605	0.56356	317.801
3.0757	0.45881	312.120
3.6908	0.36276	309.393
4.3059	0.28172	299.720
4.9210	0.21581	295.077
5.5362	0.16242	291.760
6.1513	0.12047	288.466
6.7664	0.08911	286.234
7.3816	0.06408	284.540
7.9967	0.04646	283.227


```

$JOB          PROGRAM REGENERATIVE BED HEAT CYCLING -- IMPLICIT.
$TIME        004
$TRJOB IMPDET 60
$SPECIFIC HEAT  NOLIST,NODECK
C
C  DESIGN OF REGENERATIVE BED HEAT EXCHANGER BY IMPLICIT NUMERICAL
C  APPROACH, APPLICABLE FOR BOTH HIGH AND LOW THERMAL CONDUCTIVITY
C  OF SOLID SPHERES.
C  THE RADIUS OF SOLID HAS BEEN DIVIDED INTO 5 EQUAL SEGMENTS, WHILE
C  THE REACTOR BED HAS MAXIMUM OF 100 INCREMENTS.
C  ALL INPUT DATA ARE IN 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96, 97, 98, 99, 100, 101, 102, 103, 104, 105, 106, 107, 108, 109, 110, 111, 112, 113, 114, 115, 116, 117, 118, 119, 120, 121, 122, 123, 124, 125, 126, 127, 128, 129, 130, 131, 132, 133, 134, 135, 136, 137, 138, 139, 140, 141, 142, 143, 144, 145, 146, 147, 148, 149, 150, 151, 152, 153, 154, 155, 156, 157, 158, 159, 160, 161, 162, 163, 164, 165, 166, 167, 168, 169, 170, 171, 172, 173, 174, 175, 176, 177, 178, 179, 180, 181, 182, 183, 184, 185, 186, 187, 188, 189, 190, 191, 192, 193, 194, 195, 196, 197, 198, 199, 200, 201, 202, 203, 204, 205, 206, 207, 208, 209, 210, 211, 212, 213, 214, 215, 216, 217, 218, 219, 220, 221, 222, 223, 224, 225, 226, 227, 228, 229, 230, 231, 232, 233, 234, 235, 236, 237, 238, 239, 240, 241, 242, 243, 244, 245, 246, 247, 248, 249, 250, 251, 252, 253, 254, 255, 256, 257, 258, 259, 260, 261, 262, 263, 264, 265, 266, 267, 268, 269, 270, 271, 272, 273, 274, 275, 276, 277, 278, 279, 280, 281, 282, 283, 284, 285, 286, 287, 288, 289, 290, 291, 292, 293, 294, 295, 296, 297, 298, 299, 300, 301, 302, 303, 304, 305, 306, 307, 308, 309, 310, 311, 312, 313, 314, 315, 316, 317, 318, 319, 320, 321, 322, 323, 324, 325, 326, 327, 328, 329, 330, 331, 332, 333, 334, 335, 336, 337, 338, 339, 340, 341, 342, 343, 344, 345, 346, 347, 348, 349, 350, 351, 352, 353, 354, 355, 356, 357, 358, 359, 360, 361, 362, 363, 364, 365, 366, 367, 368, 369, 370, 371, 372, 373, 374, 375, 376, 377, 378, 379, 380, 381, 382, 383, 384, 385, 386, 387, 388, 389, 390, 391, 392, 393, 394, 395, 396, 397, 398, 399, 400, 401, 402, 403, 404, 405, 406, 407, 408, 409, 410, 411, 412, 413, 414, 415, 416, 417, 418, 419, 420, 421, 422, 423, 424, 425, 426, 427, 428, 429, 430, 431, 432, 433, 434, 435, 436, 437, 438, 439, 440, 441, 442, 443, 444, 445, 446, 447, 448, 449, 450, 451, 452, 453, 454, 455, 456, 457, 458, 459, 460, 461, 462, 463, 464, 465, 466, 467, 468, 469, 470, 471, 472, 473, 474, 475, 476, 477, 478, 479, 480, 481, 482, 483, 484, 485, 486, 487, 488, 489, 490, 491, 492, 493, 494, 495, 496, 497, 498, 499, 500, 501, 502, 503, 504, 505, 506, 507, 508, 509, 510, 511, 512, 513, 514, 515, 516, 517, 518, 519, 520, 521, 522, 523, 524, 525, 526, 527, 528, 529, 530, 531, 532, 533, 534, 535, 536, 537, 538, 539, 540, 541, 542, 543, 544, 545, 546, 547, 548, 549, 550, 551, 552, 553, 554, 555, 556, 557, 558, 559, 560, 561, 562, 563, 564, 565, 566, 567, 568, 569, 570, 571, 572, 573, 574, 575, 576, 577, 578, 579, 580, 581, 582, 583, 584, 585, 586, 587, 588, 589, 590, 591, 592, 593, 594, 595, 596, 597, 598, 599, 600, 601, 602, 603, 604, 605, 606, 607, 608, 609, 610, 611, 612, 613, 614, 615, 616, 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2176, 2177, 2178, 2179, 2180, 2181, 2182, 2183, 2184, 2185, 2186, 2187, 2188, 2189, 2190, 2191, 2192, 2193, 2194, 2195, 2196, 2197, 2198, 2199, 2200, 2201, 2202, 2203, 2204, 2205, 2206, 2207, 2208, 2209, 2210, 2211, 2212, 2213, 2
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T=1
22 WRITE (6,4) TIME
4  FORMAT (1H0, 4X, 4HAI, 4X, 4H, 4X, 4H, 4X, 4H)
WRITE (6,7)
7  FORMAT (1H, 4X, 2H1, 2X, 2H2, 2X, 2H3, 2X, 2H4, 2X, 2H5, 2X, 2H6, 2X, 2H7, 2X, 2H8, 2X, 2H9, 2X, 2H10)
CALCULATION OF CONSTITUENTS IN THE MIXTURE.
50 AN=DT*2.0*(1.0-V)*F1*HF/(R*V*F*CP*DS)
    RN=F1*SV/(VF*CS*DS*DR*DS)
    CN=61.0*DR*HF/SV
    DN=992.0/(184.0+CN)
    DR=DT*RN/2.0
    F(1)=DR/9.0
    F(2)=-DR/7.50
    F(3)=-DR/10.50
    F(4)=42.0-9.0*DN
    F(5)=50.0
    F(6)=-9.0
41 A(1)=0.0
    A(2)=DR/9.0
    A(3)=-DR/5.0
    A(4)=-9.0*DR/21.0
    A(5)=50.0*DN-46.0
    A(6)=-22.0
    R(1)=1.0+1.0*DR/4.0
    R(2)=1.0+4.0*DR/3.0
    R(3)=1.0+8.0*DR/5.0
    R(4)=1.0+12.0*DR/7.0
    R(5)=270.0/DM+1410.0-22.0*DR
    R(6)=184.0+2.0*(184.0+DM)/AN
    C(1)=-27.0*DR/2.0
    C(2)=-12.0*DR/9.0
    C(3)=-19.0*DR/15.0
    C(4)=-24.0*DR/21.0
    C(5)=-DN*CN
41 C(6)=0.00
    D(1)=1(1,T)*(2.0-R(1))+F(2,T)*(-1(1))+F(3,T)*(-1(1))
    D(2)=-A(2)*1(1,T)+(2.0-R(2))*F(2,T)-1(2)*F(3,T)
    D(3)=-F(2)*1(1,T)-A(3)*F(2,T)+(2.0-R(3))*F(3,T)-1(3)*F(4,T)
    D(4)=-F(3)*1(2,T)-A(4)*F(3,T)+(2.0-R(4))*F(4,T)-1(4)*F(5,T)
    D(5)=-F(4)*1(3,T)-A(5)*F(4,T)+(270.0/DM+1410.0-22.0*DR-46.0)*F(5,T)
    D(5)=D(5)+15(1)*DN*CN
    D(6)=0.0*1(2,T)-50.0*F(4,T)+22.0*F(5,T)
    D(6)=D(6)+(2.0*(184.0+DM)/AN-184.0)*F(6,T)
    F(1)=F(1)/R(1)
    F(1)=F(1)-A(2)*F(1)
    C(1)=F(1)-A(2)*F(1)
    D(1)=D(1)-D(2)*F(1)
    F(2)=F(6)/F(4)
    F(5)=F(5)-A(5)*F(2)

```


(SAMPLE CONTINUED)

TABLE 1. REGENERATIVE EFFICIENCY OF EXCHANGER - SAMPLE 11.

AT 1.0222 MIN.

337.97	282.45	284.26	287.20	279.23	313.57
327.34	281.73	283.05	286.11	274.38	307.32
318.19	281.22	282.13	284.40	240.40	301.64
310.44	280.86	281.92	283.76	258.33	296.13
304.11	280.60	281.11	282.55	280.04	297.87
298.91	280.42	280.78	281.87	284.47	289.71
294.72	280.30	280.86	281.40	283.71	287.47
291.29	280.21	280.34	280.88	287.67	287.00
288.75	280.15	280.24	280.70	281.78	284.71
286.60	280.11	280.23	280.89	281.26	283.14
285.00	280.07	280.14	280.36	288.18	287.34
283.85	280.08	280.10	280.26	280.60	281.74
282.01	280.03	280.07	280.18	280.11	281.71

AT 2.0833 MIN.

343.74	302.44	304.18	317.24	321.25	347.70
337.26	297.83	300.74	306.40	314.81	341.06
230.81	294.10	296.50	301.62	309.14	318.72
224.61	291.10	293.71	297.56	304.73	314.03
218.70	288.00	290.47	294.18	300.77	308.10
213.41	285.19	288.26	290.30	296.43	303.80
208.55	285.28	286.47	288.11	283.41	299.67
204.21	284.07	285.07	287.25	280.88	298.00
200.30	283.16	283.97	285.75	288.80	293.47
297.05	282.44	283.08	284.54	287.01	291.15
294.18	281.87	282.33	283.57	280.88	289.07
291.72	281.43	281.85	282.80	284.38	287.35
289.64	281.09	281.42	282.07	283.54	287.33


```

$JOB          T50001 REGENERATIVE HEAT EXCHANGER - UNCOUPLING.
$TIME        004
$IRJOB FIXED  GO
$IRTC EXCHAN NO IRT,NO IRR
C
C DESIGN OF REGENERATIVE HEAT EXCHANGER WITH LOW THERMAL STRESS IN
C SOLID SPHERES - BY THE METHOD OF UNCOUPLING.
C ALL INPUT DATA ARE IN LB, HR, FT, RTD, DEG F, UNLESS SPECIFIED.
C FOR CONVERGENCE OF THE NUMERICAL INTEGRATIONS THE RADIUS HAS TO
C DIVIDED INTO 21 EQUAL SECTIONS.
C INTEGRALS ARE EVALUATED BY SIMPSON METHOD WITH TRAPZ CORRECTION.
C DIFFERENTIAL EQUATIONS ARE INTEGRATED BY RUNGE-KUTTA METHOD.
C
C GR - MASS FLOW RATE OF GAS.
C EL - LENGTH OF THE REGENERATIVE ASSEMBLY.
C TO - INITIAL TEMPERATURE OF SOLID SPHERES.
C V - FRACTIONAL VOID OF THE REGENERATIVE BED.
C AR - RADIUS OF THE SOLID SPHERE.
C DS - DENSITY OF SOLID SPHERES.
C CS - SPECIFIC HEAT OF THE SOLID SPHERES.
C HF - HEAT TRANSFER COEFFICIENT BETWEEN GAS AND SOLID SPHERES.
C SK - THERMAL CONDUCTIVITY OF SOLID SPHERES.
C CP - SPECIFIC HEAT OF GAS AT MEAN TEMPERATURE.
C DF - DENSITY OF GAS AT MEAN TEMPERATURE.
C ECT - PART OF A CYCLE REQUIRED IN THE PROGRAM IN MINUTES.
C CT - THE TIME PER CYCLE IN MINUTES.
C TG(1) - INLET GAS TEMPERATURE.
C ES - FRACTIONAL ERROR ALLOWED IN THE ENERGY BALANCE BETWEEN GAS
C AND SOLID SPHERES.
C EN1 - NO. OF INCREMENTS PER CYCLE.
C N2 - NO. OF DATA INPUT FOR ERF(X).
C N3 - 21 GIVEN DIVISIONS ALONG THE RADIUS OF SPHERE.
C N4 - NO. OF INCREMENTS ALONG THE RADIUS.
C ERF(X) - ERROR FUNCTION AT X.
C TG - GAS TEMPERATURE.
C T(J) - SOLID TEMPERATURE AT THE JTH SECTION.
C TS - SURFACE TEMPERATURE OF SOLID SPHERE.
C
C OUTPUT DATA ARE IN 7 COLUMNS OF GAS TEMPERATURE AND SOLID TEMPERATURE
C OF TG, TT, T11, T15, T19 AND SURFACE TEMPERATURE.
C
C DIMENSION TG(20), T(20,21), TT(21), R(21), ERF(21), ERF(21)
C DIMENSION ERF(21), PA(21,21), PE(21,21), X(21), ERF(21), T(21)
C DIMENSION S(4), PE(21,21)
C INPUT DATA.
C READ (5,1) GR, EL, TO, V, AR, DS, CS, HF
1  FORMAT (F8.1, F6.2, F1.1, F1.1, F7.3, F7.1, F7.3, F7.2)
C READ (5,2) SK, CP, DF, CT, ECT
2  FORMAT (F8.3, F7.3, F7.2)
C READ (5,3) TG(1), ES, EN1, N2, N3, N4
3  FORMAT (F7.1, F8.4, F8.2, I4)
C WRITE (6,84)
84  FORMAT (1H-, 10X, 2-HDATA GIVEN BELOW ARE 278 )
C WRITE (6,84)

```



```

22 IF (U-107.75.0) GO TO 24
PR(1,J)=1.0/EXP(U)
24 IF (U-101.75.0) GO TO 20
PR(1,J)=1.0/EXP(U)
20 CONTINUE
DO 116 I=1,N1
XJ=(AR-R(1))*AB
119 DO 120 J=1,N2
IF (XJ.LT.X(J)) GO TO 121
IF (XJ.EQ.X(J)) GO TO 122
120 CONTINUE
XER=1.00
GO TO 117
122 XER=1.0-ERF(J)
GO TO 117
121 DX=(XJ-X(J-1))/5.0
DO 123 JA=1,7
FJA=JA-1
XX=(X(J-1)+FJA*DX)**2
123 Y(JA)=1.0/EXP(XX)
XER=41.0*(Y(1)+Y(7))+218.0*(Y(2)+Y(6))+27.0*(Y(3)+Y(5))
XER=(XER+272.0*Y(4))*DX**2.0/(140.0*SQRT(PI))
XER=1.0-ERF(J-1)-XER
117 PER(1)=XER
116 DO 73 I=1,N1
FXA(I)=R(I)*R(I)*FXA(I)
DO 73 J=1,N1
73 PA(I,J)=(PA(I,J)-PR(1,J)-PR(1,J))*R(J)
107 IA=1
TIME=TIME+DT*60.0
WRITE (6,81) TIME
81 FORMAT (1H0, 5X, 3HAT, F9.6, 6H MIN. )
C ITERATION FOR ENTHALPY BALANCE BETWEEN THE TWO PHASES.
101 P=T(IA,N3)
TS=P4*T(IA)+18.0*T(IA,N3-1)-9.0*T(IA,N3-2)+2.0*T(IA,N3-3)
TS=TS/(11.0+B4)
Q=(TS-P)/DT
DO 30 I=1,N3
30 Y(I)=R(I)*T(IA,I)*(-PER(I))
A21=DR*2.0*(Y(27)+2.0*(Y(13)+Y(17))+4.0*(Y(11)+Y(15)+Y(19)))/3.0
A22=2.0*(Y(17)+Y(13)+Y(11)+Y(15)+Y(19))+4.0*(Y(12)+Y(14)+Y(16))
A22=DR*(A22+4.0*(Y(18)+Y(20)+Y(27)))/3.0
A23=(A22-A21)/15.0
A2=(A22+A23)/(AR*TK)
100 Q1=A1*(A2+A3*P+A4*Q)
TA=IG(IA)
DO 40 K=1,4
S(K)=H2*DT*(P+Q*DT/2.0-TA)
IF (K.GT.2) GO TO 42
TA=IG(TA)+S(K)*0.50
GO TO 40
42 IF (K.GT.4) GO TO 114

```



```

      IA=IG(IA)+C(K)
4  CONTINUE
45  IG(IA+1)=IG(IA)+(S(1)+S(4)+2.0*(S(2)+S(3)))/6.0
      Q2=(IG(IA)-IG(IA+1))*R1
      QST=Q*Q1+P
      TFS=AFS*(Q1-Q2)
      TFS=TFS*2.0/(Q1+Q2)
      IF (TFS.LE.FS) GO TO 50
54  Q=((Q1+Q2*2.0)/(2.0*A1)-A2-A3*P)/A4
      GO TO 100
50  DO 55 I=2,N3
      DO 56 J=1,N1
56  Y(J)=I(IA,J)*PA(I,J)
      W1=4.0*Y(2)
      DO 58 K=1,7,4
58  W1=W1+2.0*Y(K)+4.0*Y(K+2)
      A21=DP*2.0*(Y(1)+Y(2)+W1)/3.0
      W2=4.0*Y(2)
      DO 59 K=3,19,2
59  W2=W2+2.0*Y(K)+4.0*Y(K+1)
      A22=DP*(Y(1)+Y(2)+W2)/3.0
      A23=(A22-A21)/15.0
      IA=(A22+A23)/(2.0*R(1)*A5)
      IA1=AR*P*HF(K(J))/R(1)
      IR=(DT+(AR-R(1))*2/(TK+TK))*HF(I)
      IC=-(AR-R(1))*A6*FXC(I)
      IC1=(IR+IC)*AR*Q/R(1)
55  IT(I)=IA+IA1+IC1
      IT(1)=280.0
      WRITE (6,83) IG(IA+1), IT(3), IT(7), IT(11), IT(15), IT(19), DT
83  FORMAT (1H, 1X, F10.3, 1X, 6F10.2)
C  END OF ONE REACTOR INCREMENT CALCULATION.
      IF (IA.GE.N4) GO TO 61
60  DO 64 I=1,N3
64  T(IA,I)=IT(I)
      IA=IA+1
      GO TO 101
61  IF (TIME.LI.FCT) GO TO 102
      WRITE (6,87)
87  FORMAT (1H-, 15X, 2)END OF CALCULATION. )
      END

```

\$ENTRY	EXCHAN						
2000.0	4.68	280.0	0.345	0.050	004.6	0.191	20.00
0.100	0.220	23.00	5.00	2.00			
350.0	0.0010	48.00	21	21	13		
0.100	0.000000						
0.100	0.112463						
0.200	0.222703						
0.300	0.328627						
0.400	0.428392						
0.500	0.520500						
0.600	0.603856						
0.700	0.677801						

1.000	0.742101
1.000	0.706008
1.000	0.842701
1.200	0.010314
1.400	0.052285
1.600	0.076448
1.800	0.080091
2.000	0.095322
2.200	0.098137
2.400	0.099311
2.600	0.099764
2.800	0.000125
3.000	0.000078

(SAMPLE OUTPUT)

150001 REGENERATIVE BED HEAT EXCHANGER - DECOMPIRG.

AT 0.023222 MIN.

338.063	281.62	283.44	288.71	288.86	315.17	324.82
327.502	281.11	282.41	286.14	294.14	307.00	318.00
318.396	280.75	281.68	284.42	290.54	301.39	308.58
310.707	280.51	281.17	283.17	287.82	296.46	302.71
304.326	280.34	280.81	282.26	285.11	292.67	297.87
299.107	280.23	280.56	281.61	284.24	289.58	293.64
294.892	280.15	280.38	281.14	283.10	287.25	290.52
291.525	280.10	280.26	280.81	282.26	285.45	288.05
288.861	280.06	280.18	280.57	281.64	284.08	286.14
286.112	280.04	280.12	280.40	281.14	283.04	284.61
285.147	280.02	280.08	280.28	280.76	282.27	283.11
282.892	280.01	280.05	280.15	280.62	281.66	282.61
282.452	270.00	280.00	270.00	280.00	281.24	281.01

AT 2.083222 MIN.

343.707	307.89	309.21	311.78	320.67	331.24	336.60
337.220	297.32	300.21	306.08	314.41	324.53	327.58
330.791	293.63	296.17	301.26	308.90	318.33	323.68
324.609	290.68	292.84	297.23	305.33	312.72	317.32
318.802	288.33	290.13	293.89	299.15	307.11	312.41
313.454	286.46	287.77	291.33	296.20	303.30	307.65
308.607	285.00	286.24	288.88	293.21	298.45	303.38
304.270	283.85	284.86	287.05	290.00	295.84	299.63
300.462	282.06	283.13	284.98	286.64	293.31	286.78
297.131	282.26	282.72	284.37	286.00	293.82	284.21
294.256	281.12	282.29	283.44	285.76	288.00	283.47
291.775	281.31	281.73	282.66	284.43	286.23	280.20
287.422	284.00	287.33	287.40	280.00	281.00	284.00


```
$ JOB          150001  ACETYLENE PRODUCTION BY DECOUPLING.
$ TIME          006
$ PROBLEM FUND  60
$ INPUT FINAL   NO LIST, NO DECK
(
(
(   THIS PROGRAM IS DEVELOPED IN ACCORDING TO THE DEGENERATIVE
(   HEAT EXCHANGER DECOUPLING TECHNIQUE, AND IS HEREIN
(   APPLIED TO THE PRODUCTION OF ACETYLENE FROM METHANE.
(   ALL INPUT DATA ARE IN IN, HP, FT, HDO, DEG F, W/HR SPECIFIED.
(
(   SK - THERMAL CONDUCTIVITY OF SOLID SPHERES.
(   CS - SPECIFIC HEAT OF SOLID SPHERES.
(   DS - DENSITY OF SOLID SPHERES.
(   AR - RADIUS OF SOLID SPHERE IN INCHES.
(   HF - HEAT TRANSFER COEFFICIENT BETWEEN GAS AND SOLID SPHERE.
(   AS - TOTAL SURFACE AREA OF SOLID SPHERES PER UNIT VOLUME (PA).
(   V - FRACTIONAL VOID OF THE REACTOR BED.
(   GF - MASS FLOW RATE OF GAS.
(   CP1, CP2, CP3 - MOLAR SPECIFIC HEAT OF METHANE, ACETYLENE,
(   AND HYDROGEN RESPECTIVELY.
(   FL - LENGTH OF THE REACTOR BED.
(   TR - BASE TEMPERATURE.
(   HR - HEAT OF REACTION AT TEMPERATURE TR.
(   TGO - INLET GAS TEMPERATURE.
(   TO - INITIAL SOLID TEMPERATURE.
(   PO - INLET TOTAL PRESSURE.
(   XO - INLET FRACTIONAL CONVERSION OF FEED.
(   DT - THE TIME PER CYCLE IN MINUTES.
(   FCT - PART OF A CYCLE REQUIRED IN THE PROGRAM IN MINUTES.
(   FE - FRACTIONAL ERROR ALLOWED IN THE ENERGY BALANCE BETWEEN GAS
(   AND SOLID SPHERES.
(   N2 - NO. OF DATA INPUT FOR PRE(X).
(   N3 - NO. OF DIVISIONS IN THE RADII VARIABLE.
(   N4 - NO. OF INCREMENTS ALONG THE REACTOR BED.
(
(   DIMENSION T(25,17), TI(17), F(17), FXA(17), CX(17), DE(17)
(   DIMENSION PA(17,17), PR(17,17), PE(17,17), X(20), FFE(20), Y(17)
(   DIMENSION TY(3), S(3,4), F(3)
1  FORMAT (2X, F6.4, F8.4, F8.2, F6.2, F1.2, F1.2, F1.4)
2  FORMAT (2X, F6.2, F8.4, F8.4, F9.2, F1.2, F3.4, F8.4)
3  FORMAT (2X, F7.2, F9.2, F3.2, F6.2, F1.2, F1.2)
4  FORMAT (1X, F7.4, 4I4)
5  FORMAT (1X, F6.3, 2X, F8.6)
81  FORMAT (1H0, 5X, 4FAT, F1.6, 6H ATN. )
82  FORMAT (1H, 3X, F15.8, 5X, F15.2, 5X, F15.8, 5X, F15.8)
83  FORMAT (1H, 2X, 6F10.2)
84  FORMAT (1H-, 1X, 28HDATA GIVEN BELOW (SEE FEED )
85  FORMAT (1H0, 5X, 4H1(3), 6X, 4H1(7), 5X, 6H1(N-6), 4X, 6H1(N-4),
(   14X, 6H1(N-2), 6X, 2H1( )
86  FORMAT (1H0, 10X, 2HIG, 18X, 1H0, 1X, 1H, 1X, 1H )
(   READ (5,1) SK, CS, DS, AR, HF, AS, V
(   READ (5,2) GF, CP1, CP2, CP3, FL, TR, HR
(   READ (5,3) TGO, TO, PO, XO, DT, FCT
```



```

      READ (5,4) F5, N2, N3, N4
      READ (5,5) (X(J), FPF(J), J=1,N2)
      WRITE (6,84)
      WRITE (6,85)
      WRITE (6,86)
      AR=AR/12.0
      FN3=NX-1
      N3A=NX-2
      N3B=NX-4
      DR=AR/FN3
      FN4=N4
      N4A=N4+2
      DZ1=F1/FN4
      GR=10.78*1.80
      DI=DI/3600.0
      HR=HR*1000.0
      FIF=50.0
      TIME=0.00
      TK=SK/(DS*CS)
      PT=3.141593
      AA1=3.0*SK*(1.0-V)/AR
      A6=SQRT(DI/(PT*TK))
      A3=-DI/AR+2.0*A6
      A4=-DI*DI/(2.0*AR)+4.0*DI*A6/2.0
      A5=SQRT(DI*PT*TK)
      A7=1.0/(4.0*TK*DI)
      A8=1.0/(2.0*SQRT(TK*DI))
      B1=HF*AS/GF
      R2=0.5*(P2+1.5*(P3-(P1
      R3=V/(GR*GF)
      R4=12.0*DR*HF/SK
      R5=0.000835
      R6=12.826
      R7=10214.
      R8=4.358
      R9=5002.0
      DO 9 I=1,N4A
      DO 9 J=1,N3
9      T(I,J)=T0
      DO 10 I=1,N2
      FI=I-1
10      R(I)=FI*DR
      DO 11 I=1,N3
      EXA(I)=0.00
      EXC(I)=0.00
      DO 11 J=1,N4
      PA(I,J)=0.00
      PE(I,J)=0.00
11      PR(I,J)=0.00
      DO 13 I=1,N3
      UA=R(I)*R(I)*A7
      UC=(AR-R(I))*2*A7
      IF (UA.GT.FIF) GO TO 17
```



```

      EXA(I)=1.0/EXP(UA)
117  IF (UC.GT.FIF) GO TO 118
      EX(I)=1.0/EXP(UC)
118  CONTINUE
      DO 20 I=1,N3
      DO 20 J=1,N3
      UA=(R(I)-R(J))**2*A7
      UB=(R(I)+R(J))**2*A7
      UF=(-2.0*AR+R(I)+R(J))**2*A7
      IF (UA.GT.FIF) GO TO 22
      PA(I,J)=1.0/EXP(UA)
22  IF (UB.GT.FIF) GO TO 24
      PB(I,J)=1.0/EXP(UB)
24  IF (UF.GT.FIF) GO TO 20
      PF(I,J)=1.0/EXP(UF)
20  CONTINUE
      DO 116 I=1,N3
      XJ=(AP-R(I))*AR
119  DO 120 J=1,N2
      IF (XJ.LT.X(J)) GO TO 121
      IF (XJ.EQ.X(J)) GO TO 122
120  CONTINUE
      XFR=0.0
      GO TO 117
122  XFR=1.0-FRF(J)
      GO TO 117
121  DX=(XJ-X(J-1))/6.0
      DO 123 JA=J,7
      FJA=JA-1
      XX=(X(J-1)+FJA*DX)**2
124  Y(JA)=1.0/EXP(XX)
      XFR=41.0*(Y(1)+Y(7))+216.0*(Y(2)+Y(6))+27.0*(Y(4)+Y(3))
      XFR=(XFR+272.0*Y(4))*DX*2.0/(140.0*SQRT(PJ))
      XFR=1.0-FRF(J-1)-XFR
117  FRF(I)=XFR
116  CONTINUE
      DO 73 I=1,N3
      EXA(I)=R(I)*R(I)*EXA(I)
      DO 73 J=1,N3
73  PA(I,J)=(PA(I,J)+PB(I,J)+PF(I,J))*U(J)
102  IA=1
      TIME=TIME+DT*60.0
      WRITE(6,81) TIME
      XI=0.0
      IY(1)=TGO
      IY(2)=XO
      IY(3)=PO
103  P=1/(IA*N3)
      IF (IA.GT.4) GO TO 76
      IF (IA.EQ.4) GO TO 75
      DZ=DZ1*(0.2)
      GO TO 101
75  DZ=DZ1*0.40

```



```

30  DO 10 I=1,N
10  DZ=DZ/L
101  A1=AA1*DZ
      TS=H4*Y(1)+(8.0)*I*(1A*N3-1)-7.0*I*(1A*N3-2)+2.0*I*(1A*N3-3)
      TS=TS/(11.0+4)
      O=(TS-D)/D1
      DO 30 I=1,N2
30  Y(I)=R(I)*I*(1A.1)*(-H4*O(I))
      W1=4.0*Y(3)
      DO 301 K=5,N3H,4
301  W1=W1+2.0*Y(K)+4.0*Y(K+2)
      A21=DZ*2.0*(Y(1)+Y(N3)+W1)/3.0
      W2=4.0*Y(2)
      DO 302 K=1,N3A,2
302  W2=W2+2.0*Y(K)+4.0*Y(K+1)
      A22=DZ*(Y(1)+Y(N3)+W2)/3.0
      A23=(A22-A21)/15.0
      A2=(A22+A23)/(A2*1K)
      C5=((1.0-F(2))*CP1+0.5*F(2)*CP2+1.5*F(2)*CP3)*(TY(1)-1.0)
100  Q1=A1*(A2+A2*P+A4*O)
      F(1)=TY(1)
      F(2)=TY(2)
      F(3)=TY(3)
      DO 40 K=1,4
      (1)=(1.0-F(2))*EXP(P6-P7/F(1))
      (2)=0.5*F(2)*EXP(P8-39/F(1))
      (3)=(1.0-F(2))*CP1+0.5*F(2)*CP2+1.5*F(2)*CP3
      S(2,K)=H3*OZ*F(3)*((1-(2)*4600.0)/(F(1)*(1.0+F(2))))
      S(1,K)=DZ*(P1*(P+Q*0.5*O)-F(1))-(H2*(F(1)-F(3))+H4)*S(2,K)/0.3
      S(3,K)=DZ*(1.0+F(2))*F(1)*H5/F(3)
      IF (K.GT.2) GO TO 42
      F(1)=TY(1)+S(1,K)/2.0
      F(2)=TY(2)+S(2,K)/2.0
      F(3)=TY(3)+S(3,K)/2.0
      GO TO 40
42  IF (K.GT.3) GO TO 44
      F(1)=TY(1)+S(1,K)
      F(2)=TY(2)+S(2,K)
      F(3)=TY(3)+S(3,K)
      GO TO 40
40  CONTINUE
44  DO 45 I=1,3
45  F(I)=TY(I)+(S(1,1)+S(1,4)+2.0*(S(1,2)+S(1,3)))/6.0
      C4=((1.0-F(2))*CP1+0.5*F(2)*CP2+1.5*F(2)*CP3)*(TY(1)-1.0)
      Q2=-GF*O1*(C4-C5+(F(2)-TY(2))*H4)
      FTS=ABS(Q1-Q2)
      AQ=ABS(Q1+Q2)
      FTS=FTS*2.0/AQ
      IF (FTS.LT.F5) GO TO 50
      Q=((Q1+Q2*2.0)/(4.0*AT)-A2-A3*P)/A4
      GO TO 100
50  DO 55 I=2,N2
      DO 56 J=1,N2

```



```

56  Y(J)=I(IA,J)*P(R(I,J))
    W1=4.*Y(1)
    DO 58 K=5,N2-4
58  W1=W1+2.*Y(K)+4.*Y(K+1)
    A21=DP*Z.*(Y(1)+Y(N2)+W1)/2.
    W2=4.*Y(2)
    DO 59 K=3,N2-3
59  W2=W2+2.*Y(K)+4.*Y(K+1)
    A22=DP*(Y(1)+Y(N2)+W2)/2.
    A23=(A22-A21)/15.
    IA=(A22+A23)/(2.0*R(1)*AN)
    TAI=AR*P*F(R(1)/r(1))
    TH=(D1+(AR-F(1))*Z/(1.5+1.5))*F(R(1))
    IC=-(AR-F(1))*A6*FX(1)
    TC1=(TH+IC)*AP*Q/R(1)
55  TT(J)=IA+TAI+TC1
    TT(1)=14.0
    TY(1)=F(1)
    TY(2)=F(2)
    TY(3)=F(3)
    DST=Q*DT+P
    XL=XL+DZ
    WRITE (6,83) TT(3), TT(7), TT(N3-6), TT(N3-4), TT(N3-2), DST
    WRITE (6,82) TY(1), TY(2), TY(4), XL
    IF (IA.GE.N4A) GO TO 61
    DO 64 I=1,N2
64  T(IA,I)=TT(I)
    IA=IA+1
    GO TO 103
61  IF (TIME.LT.ECT) GO TO 102
    CONTINUE
    END

```

SENTRY	FINAL
4.860	0.4932 221.88 0.50 83.00 6.80 0.400
20.00	38.880 33.696 14.112 3.00 1673.0 26.674
940.00	2000.00 15.00 7.50 5.00 3.00
0.0100	21 17 12
0.000	0.000000
0.100	0.112463
0.200	0.222703
0.300	0.328627
0.400	0.428392
0.500	0.520500
0.600	0.602856
0.700	0.677801
0.800	0.742101
0.900	0.796908
1.000	0.842701
1.200	0.910314
1.400	0.952285
1.600	0.976348
1.800	0.989091
2.000	0.995322

2.200 0.000121
 2.400 0.000111
 2.600 0.000164
 2.800 0.000125
 3.000 0.000178

(SAMPLE OUTPUT)

(SCOUT ACETYLENE PROBE FLUX BY DECOUPLING).

DATA GIVEN BELOW ARE FOR

I(2)	I(1)	I(N-6)	I(N-4)	I(N-2)	TS
IG	X		P		I
AT 2.000000 MIN.					
1086.30 1078.51	1062.42	1082.32	1041.00	1028.31	0.0500
0.07438720E+03	0.21828187E+04		0.1497332E+02		
1171.02 1160.33	1139.94	1125.95	111.56	1094.83	0.1000
0.10211317E+04	0.01168606E+05		0.14944540E+02		
1255.71 1243.32	1219.46	1205.65	0.185.75	1263.40	0.1500
0.10773338E+04	0.12911243E+04		0.14931621E+02		
1384.62 1371.04	1344.62	1326.50	133.6.40	1292.30	0.2000
0.12060508E+04	0.14290493E+03		0.14985033E+02		
1677.40 1667.36	1647.45	1633.84	1617.86	1599.14	0.2500
0.13040656E+04	0.10055931E+00		0.14963238E+02		
1772.83 1764.87	1744.10	1732.38	1727.62	1710.63	0.3000
0.15449504E+04	0.18481098E+00		0.14934418E+02		
1837.00 1830.88	1818.84	1810.00	1800.62	1785.16	0.3500
0.16549527E+04	0.25386908E+03		0.14909401E+02		
1879.77 1875.08	1865.89	1853.51	1851.41	1843.07	0.4000
0.17457356E+04	0.3122254E+00		0.14833226E+02		
1908.45 1904.80	1897.75	1892.76	1896.88	1880.02	0.4500
0.18093176E+04	0.26419067E+00		0.14842877E+02		
1928.35 1925.44	1919.83	1917.42	1911.25	1908.81	0.5000
0.18535270E+04	0.41783218E+00		0.14806909E+02		
1942.44 1940.07	1935.55	1932.42	1928.66	1924.28	0.5500
0.18861807E+04	0.45619823E+00		0.14767817E+02		
1952.69 1950.73	1947.03	1944.46	1941.38	1931.73	0.6000
0.19098526E+04	0.42750209E+00		0.1472305E+02		
1960.37 1958.71	1955.63	1952.48	1950.41	1947.32	0.6500
0.19271947E+04	0.53575371E+00		0.1468558E+02		
1966.27 1964.85	1962.24	1960.42	1960.25	1959.1	0.7000
0.19400840E+04	0.57095050E+00		0.14642525E+02		
1970.13 1969.33	1972.28	1970.39	1975.83	1973.66	0.7500
0.19640061E+04	0.60830810E+00		0.14605884E+02		

PART TWO

CORRELATION OF MULTIVARIATE DATA

I. INTRODUCTION

The task of finding suitable approximating functions may arise both in data correlation and in data representation. It is assumed that the approximating function is a linear combination of a set of specified functions and that the coefficients are to be determined using some criteria of best fit.

For data correlation, the form of the functions may be known but the data points which are to be fitted may contain errors, where these errors are randomly distributed. Then the criterion of least squares is normally used.

For the data representation the data points are assumed to be free of error and our task is to find an analytical approximating function, which may be more convenient for computational purposes. In this case, the Chebyshev criterion may be more appropriate as a criterion of best fit.

In general the problem may be stated as follows:

It is desired to approximate a real-valued function u_i by $n+1$ known functions of $g_j(x_i, y_i, z_i, \dots)$ for $0 \leq j \leq n$, at a set of points (x_i, y_i, z_i, \dots) for $i = 1, 2, \dots, m$, continuous on a closed region R . If the deviation at each point is defined as

$$\epsilon_i = u_i - \sum_{j=0}^n A_j g_j(x_j, y_j, z_j, \dots) \quad (I.1)$$

where $x, y, z \in R$

then A_j are the $n+1$ expansion coefficients to be evaluated according to the following criteria:

1. least squares criterion

$$\text{i.e. } \sum_{i=1}^m \epsilon_i^2 \quad \text{is a minimum}$$

- and
2. Chebyshev criterion

$$\text{i.e. } \epsilon_i \max_i \quad \text{is a minimum,}$$

These are by no means the only criteria for approximation. Indeed there has been considerable work done in developing the "Least Qth" method(1), for which the "least squares" is but a special case. If we define the function S by

$$S = \sum_{i=1}^m \epsilon_i^{2q} \quad (q \text{ integer}) \quad (\text{I.2})$$

and it has only one real minimum, then it is required to find the expansion coefficients A_j in minimizing S . When q is any integer other than one, the system becomes implicit in A_j so that the method of steepest ascent or other trial-and error approaches must be used in solving the problem. The complexity and the often slow rate of convergence are the drawbacks in rendering the criterion of "least Qth" rather unpopular.

When q is sufficiently large it can be seen that the criterion of "least Qth" approaches that of Chebyshev approximation in minimizing the maximum deviation.

II. CURVE FITTING BY LEAST SQUARES CRITERION

The least squares principle, originally proposed by Gauss, postulates that the best fit occurs when

$$S = \sum_{i=1}^m w_i \cdot \epsilon_i^2 \quad (\text{II.1})$$

is a minimum, where w_i is the weighting factor associated with each data point. For a function of an independent variable x , to be approximated by some general polynomials $G_j(x)$, at most of degree j , equation (II.1) may be written as

$$S = \sum_{i=1}^m w_i \left\{ u_i - \sum_{j=0}^n A_j G_j(x_i) \right\}^2 \quad (\text{II.2})$$

Since S is a quadratic function of A_j , its minimum exists at

$$\frac{\partial S}{\partial A_j} = 0 \quad \text{for } j = 0, 1, \dots, n, \quad (\text{II.3})$$

After expansion it yields

$$\begin{aligned} & \sum_{j=0}^n A_j \sum_{i=1}^m w_i \cdot G_j(x_i) \cdot G_k(x_i) \\ &= \sum_{i=1}^m w_i u_i G_k(x_i) \end{aligned} \quad (\text{II.4})$$

$k = 0, 1, 2, \dots, n.$

If we let

$$D_{jk} = \sum_{i=1}^m w_i \cdot G_j(x_i) \cdot G_k(x_i) \quad (\text{II.5})$$

and

$$E_k = \sum_{i=1}^m w_i \cdot G_k(x_i) \cdot u_i$$

then equation (II.4) can be written algebraically as

$$DA = E \quad (\text{II.6})$$

This is a system of $n+1$ linear equations. When the matrix D is non-singular it follows that A_j is unique for minimizing S . The evaluation of A_j in equation (II.6) can be achieved by any standard method in the field of linear algebra.

To check the closeness of fit, the criterion of variance δ may be used, which is defined as

$$\delta = \frac{\sum_{i=1}^m \epsilon_i^2}{m - n} \quad (\text{II.7})$$

The variance is a measure of the average deviation of the experimental points from the approximating function. The degree of the polynomial ^{is} n arbitrarily chosen at some appropriate level, however, it must be less than m . In going through

the analysis, the variance is calculated. Then n is increased by one and the analysis is repeated, until there is no significant change in the variance. However, a complete set of calculations has to be carried out for each additional polynomial tested; and the sets of expansion coefficients determined bear no relationship to the others. Furthermore, computational difficulties arise from the fact that the matrix D , in most cases, is ill-conditioned - because of the sensitivity of A_j to slight change of values in D .

The solution to both these problems - the ill conditioned matrix and the necessity for recalculating the coefficients for each higher degree polynomial tested - lies in the use of orthogonal polynomials.

When a sequence of polynomials $\{G_j(x)\}$ is orthogonal in the summation sense over a point set, they satisfy the following,

$$\sum_{i=1}^m w_i \cdot G_j(x_i) \cdot G_k(x_i) = 0 \quad j \neq k$$

$$= \sum_{i=1}^m w_i \cdot G_j^2(x_i) \quad j = k. \quad (\text{II.8})$$

When this is substituted into equation (II.4) the expansion coefficients can be evaluated very easily as

$$A_j = \frac{\sum_{i=1}^m w_i \cdot u_i \cdot G_j(x_i)}{\sum_{i=1}^m w_i \cdot G_j^2(x_i)} \quad (\text{II.9})$$

without the necessity of matrix manipulation. Furthermore, the coefficients are independent of one another and of the value n .

With the orthogonality of (II.8) and the expression (II.9), equation (II.2) yields

$$\begin{aligned} S &= \sum_{i=1}^m w_i \left\{ u_i^2 - 2u_i \sum_{j=0}^n A_j G_j(x_i) \right. \\ &\quad \left. + \sum_{j=0}^n A_j G_j(x_i) \sum_{k=0}^n A_k G_k(x_i) \right\} \\ &= \sum_{i=1}^m w_i u_i^2 - 2 \sum_{j=0}^n A_j \sum_{i=1}^m w_i u_i G_j(x_i) \\ &\quad + \sum_{j=0}^n \sum_{k=0}^n A_j A_k \sum_{i=1}^m w_i G_j(x_i) \cdot G_k(x_i) \\ &= \sum_{i=1}^m w_i u_i^2 - 2 \sum_{j=0}^n A_j^2 \sum_{i=1}^m w_i G_j^2(x_i) \end{aligned}$$

$$\begin{aligned}
& + \sum_{j=0}^n A_j^2 \sum_{i=1}^m w_i G_j^2(x_i) \\
& = \sum_{i=1}^m w_i u_i^2 - \sum_{j=0}^n A_j^2 \sum_{i=1}^m w_i G_j^2(x_i) \quad (\text{II.10})
\end{aligned}$$

Since S , by definition, is positive definite, as n increases S must decrease. This verifies the convergence of the approximation.

The literature on the subject of orthogonal polynomials is voluminous. However, we need be concerned with only certain properties. Thus, all orthogonal polynomials satisfy the recurrence formula(2).

$$\begin{aligned}
P_{n+1}(x) &= (A_n x + B_n) P_n(x) - C_n P_{n-1}(x) \\
n &= 1, 2, 3 \dots \quad (\text{II.11})
\end{aligned}$$

where A_n , B_n , C_n are arbitrarily constants to be constructed. In the following calculation A_n is taken to be unity as suggested by Forsythe(3), so that the complete recurrence form is expressed as follows:

$$\begin{aligned}
P_0(x) &= 1 \\
P_1(x) &= (x - \alpha_1) P_0(x) \\
P_2(x) &= (x - \alpha_2) P_1(x) - \beta_2 P_0(x) \\
&\dots \\
P_j(x) &= (x - \alpha_j) P_{j-1}(x) - \beta_j P_{j-2}(x)
\end{aligned} \tag{II.12}$$

where α_j, β_j are defined as follows:

$$\alpha_j = \frac{\sum_{i=1}^m w_i x_i P_{j-1}^2(x_i)}{\sum_{i=1}^m w_i P_{j-1}^2(x_i)} \tag{II.13a}$$

$$\beta_j = \frac{\sum_{i=1}^m w_i x_i P_{j-1}(x_i) \cdot P_{j-2}(x_i)}{\sum_{i=1}^m w_i P_{j-2}^2(x_i)} \tag{II.13b}$$

They can therefore be calculated sequentially in a systematic manner. Their derivation and proof of orthogonality are given in Appendix A.

An advantage of constructing such^a polynomial over other orthogonal polynomials such as Chebyshev, Gram, Laguerre and many others, is that it does not require specified spacing of the data points.

A study of the effect of weighting factors has also been investigated. By modifying the weighting factors linearly according to the absolute deviations obtained in the analysis using equal weighting factors, it was found that the maximum deviation, though not necessarily the variance, can be reduced.

Numerical illustrations are given in a later section.

III. SURFACE FITTING BY LEAST SQUARES CRITERION

This is an extension of curve fitting in section II. Here we try to find the approximating function for systems with two independent variables. The approximating function to be investigated is a mixed polynomial of the form:

$$f(x, y) = \sum_{i=0}^n \sum_{j=0}^m A_{ij} \cdot P_i(x) \cdot Q_j(y) \quad (\text{III.1})$$

where n, m are the highest degree of the polynomials in x and y , respectively.

$P(x), Q(y)$ are the orthogonal polynomials to be generated from given data through recurrence formulas as shown below:

At $y = \text{constant}$

$$\begin{aligned} P_0(x) &= 1 \\ P_1(x) &= (x - \alpha_1) P_0(x) \\ P_2(x) &= (x - \alpha_2) P_1(x) - \beta_2 P_0(x) \\ &\dots \\ P_i(x) &= (x - \alpha_i) P_{i-1}(x) - \beta_i P_{i-2}(x) \end{aligned} \quad (\text{III.2})$$

and at $x = \text{constant}$

$$\begin{aligned} Q_0(y) &= 1 \\ Q_1(y) &= (y - \gamma_1) Q_0(y) \\ Q_2(y) &= (y - \gamma_2) Q_1(y) - \delta_2 Q_0(y) \\ &\dots \\ Q_j(y) &= (y - \gamma_j) Q_{j-1}(y) - \delta_j Q_{j-2}(y), \end{aligned} \quad (\text{III.3})$$

If the data point at (x_k, y_l) is $z_{k,l}$, then the error of approximation is given by

$$\epsilon_{k,l} = z_{k,l} - f(x_k, y_l). \quad (\text{III.4})$$

For a rectangular network with u and v numbers of points along the x and y axes respectively, the sum of the error squares becomes

$$S = \sum_{k=1}^u \sum_{l=1}^v (\epsilon_{k,l})^2 \quad (\text{III.5})$$

$$= \sum_{k=1}^u \sum_{l=1}^v \left\{ z_{kl} - \sum_{i=0}^n \sum_{j=0}^m A_{ij} P_j(x_k) Q_j(y_l) \right\}^2$$

Here weighting factors are not considered and S is a function only of A_{ij} . By the criterion of least squares, it is necessary to find the matrix (A_{ij}) such that

$$\frac{\partial S}{\partial A_{st}} = 0 \quad \text{for} \quad \begin{array}{l} s = 0, 1, \dots, n \\ t = 0, 1, \dots, m. \end{array} \quad (\text{III.6})$$

After expanding equation (III.6) and rearranging, this gives

$$\begin{aligned}
& \sum_{i=0}^n \sum_{j=0}^m A_{ij} \sum_{k=1}^u \sum_{l=1}^v P_i(x_k) P_s(x_k) Q_j(y_l) Q_t(y_l) \\
&= \sum_{k=1}^u \sum_{l=1}^v z_{kl} P_s(x_k) Q_t(y_l) \quad (\text{III.7})
\end{aligned}$$

Now if $P_i(x)$ $Q_j(y)$ are orthogonal polynomials in the summation sense, i.e.

$$\begin{aligned}
& \sum_{k=1}^u \sum_{l=1}^v P_i(x_k) P_s(x_k) Q_j(y_l) Q_t(y_l) \\
&= 0 \quad \text{if } i \neq s \quad \text{or } j \neq t \\
&\text{but} \\
&= \sum_{k=1}^u \sum_{l=1}^v P_s^2(x_k) Q_t^2(y_l) \quad \text{if and only if} \\
&\quad \quad \quad s = i \quad \text{and} \\
&\quad \quad \quad t = j \quad (\text{III.8})
\end{aligned}$$

then the expansion coefficients can readily be evaluated as

$$A_{ij} = \frac{\sum_{k=1}^u \sum_{l=1}^v z_{kl} P_i(x_k) Q_j(y_l)}{\sum_{k=1}^u \sum_{l=1}^v P_i^2(x_k) Q_j^2(y_l)} \quad (\text{III.9})$$

It has been proved in Appendix B that if

$$\alpha_i = \frac{\sum_{k=1}^u x_k P_{i-1}^2(x_k)}{\sum_{k=1}^u P_{i-1}^2(x_k)} \quad (\text{III.10a})$$

$$\beta_i = \frac{\sum_{k=1}^u x_k P_{i-1}(x_k) P_{i-2}(x_k)}{\sum_{k=1}^u P_{i-2}^2(x_k)} \quad (\text{III.10b})$$

$$\gamma_j = \frac{\sum_{l=1}^v y_l Q_{j-1}^2(y_l)}{\sum_{l=1}^v Q_{j-1}^2(y_l)} \quad (\text{III.10c})$$

and

$$\delta_j = \frac{\sum_{l=1}^v y_l Q_{j-1}(y_l) Q_{j-2}(y_l)}{\sum_{l=1}^v Q_{j-2}^2(y_l)} \quad (\text{III.10d})$$

then $P_i(x_k) Q_j(y_l)$ will indeed satisfy the orthogonality condition of (III.8)

The application of this analysis has given very satisfactory results in comparison with that using Chebyshev polynomials. However, there is difficulty in incorporating any weighting factors. Furthermore, this approach requires the data points to be on a rectangular grid.

IV. FUNCTION APPROXIMATION BY CHEBYSHEV CRITERION

The statement of the problem is as follows: Given a set of real functional values $f(x)$ at $x = x_i$, ($i = 1, 2, \dots, m$) and $n+1$ known functions $g_j(x)$ for $0 \leq j \leq n$, continuous on a closed region R , find an $n+1$ dimensional real vector $\alpha = (\alpha_j)$ such that the norm of

$$\lambda = f(x) - \sum_{j=0}^n \alpha_j g_j(x) \quad x \in R \quad (IV.1)$$

is a minimum.

This problem can be solved by some iterative method(4), based upon the theorem of de la Vallie Poussin(5), which states that

(i) The solution vector α_j which furnishes the best approximation to (IV.1) gives at least $n+1$ residuals equal to $\pm M$,

$$\text{where } M = \min_{\alpha_j} \left\{ \left| f(x_i) - \sum_{j=0}^n \alpha_j g_j(x_i) \right|_{\max_i} \right\}$$

(ii) The minimal-maximum residual M of a system of m linear equations in $n+1$ unknowns is equal to the largest of the minimal-maximum residuals M_1, M_2, \dots corresponding to the various systems which can be found in taking $n+2$ equations at a time.

In general the method can be described as follows:

1. choose arbitrarily $n+2$ points $f(x_i)$ with $x_i \in R$, forming a set of $n+2$ simultaneous equations,
2. solve the simultaneous equations to yield $\alpha_j^{(1)}$ and $\lambda^{(1)}$ (where the superscripts represent the number of trials),
3. find a point $f(x_r)$ in R other than those in the set

$$\exists \quad \left| f(x_r) - \sum_{j=0}^n \alpha_j g_j(x_r) \right| > \lambda^{(1)},$$

4. replace one of the points $f(x_i)$ by $f(x_r)$ to form a new set,
5. now repeat the calculations until

$$\left| f(x_i) - \sum_{j=0}^n \alpha_j g_j(x_i) \right| < \lambda \quad \text{for } i = 1, 2, \dots, m.$$

At worst this method requires a selection and solution of $\binom{m}{n+2}$ systems of $n+2$ equations in $n+2$ unknowns. When m is large, which is usually the case, the method becomes so time consuming as to be impractical.

Since the problem is to find the minimum λ subject to

$$\left| f(x_i) - \sum_{j=0}^n \alpha_j g_j(x_i) \right| \leq \lambda \quad 1 \leq i \leq m$$

i.e.

$$\begin{aligned}\lambda + \sum_{j=0}^n \alpha_j g_j(x_i) &\leq f(x_i) \\ \lambda - \sum_{j=0}^n \alpha_j g_j(x_i) &\leq -f(x_i)\end{aligned}\tag{IV.2}$$

it can be framed as a linear programming problem.

V. LINEAR PROGRAMMING - SIMPLEX METHOD

It is appropriate here to give a brief description of linear programming and its solution by the Simplex method. Detailed discussion of the method can be found in many standard textbooks(6,7,8).

The general linear programming problem is to find a vector $\alpha = \alpha(\alpha_1, \alpha_2, \dots, \alpha_n)$ which minimizes the linear form (i.e. the objective function)

$$\sum_{j=1}^n c_j \alpha_j = B \quad (V.1a)$$

subject to the linear constraints

$$\alpha_j \geq 0 \quad j = 1, 2, \dots, n \quad (V.1b)$$

and

$$\sum_{j=1}^n a_{ij} \alpha_j = b_i \quad i = 1, 2, \dots, m \quad (V.1c)$$

where the a_{ij} , b_i and c_j are given constants and $n < m$.

If the constraints involve inequalities, slack variables s_i are introduced.

Therefore,

$$a_{i1}\alpha_1 + a_{i2}\alpha_2 + \dots + a_{in}\alpha_n \leq b_i$$

may be written as

$$a_{i1}\alpha_1 + a_{i2}\alpha_2 + \dots + a_{in}\alpha_n + s_i = b_i$$

where s_i is non-negative.

If some variables are not constrained to be non-negative then it is necessary to let

$$\alpha_j = \alpha_j^{(1)} - \alpha_j^{(2)}$$

because any number can always be expressed as the difference of two non-negative numbers.

If the objective function is required to be maximized

i.e.
$$\sum_{j=1}^n c_j \alpha_j = \max.$$

it can be rewritten as

$$- \sum_{j=1}^n c_j \alpha_j = \min.$$

By arithmetic manipulation the given system (IV.1) can readily be transformed into a canonical form as

$$\begin{aligned} \alpha_1 &+ a'_{1,m+1} \alpha_{m+1} + \dots + a'_{1,n} \alpha_n = b'_1 \\ \alpha_2 &+ a'_{2,m+1} \alpha_{m+1} + \dots + a'_{2,n} \alpha_n = b'_2 \\ &\dots \dots \dots \\ \alpha_m &+ a'_{m,m+1} \alpha_{m+1} + \dots + a'_{m,n} \alpha_n = b'_m \\ &c'_{m+1} \alpha_{m+1} + \dots + c'_n \alpha_n = B - B_0 \end{aligned} \tag{V.2}$$

where B_0 is a constant.

Here $\alpha_1, \alpha_2, \dots, \alpha_m$ are the basic variables.

Hence, the canonical form for any basis is the rearrangement of the original system so that the variables become unit vectors.

The Simplex method is an iterative procedure which searches for the optimum from one basic feasible solution to another basic feasible solution, having a lower value of B . Thus, the Simplex method deals only with the canonical form of bases and consists of the following steps:

1. examine the c'_j and find the smallest one (say) c'_s ,
2. if $c'_s \geq 0$, then the current solution is optimal,
3. if $c'_s < 0$, from the column of coefficients a'_{is} pick out those $a'_{is} > 0$,
4. if all $a'_{is} \leq 0$, then no unique optimal solution exists,
5. if some $a'_{is} > 0$, find the i for which b'_i/a'_{is} is the smallest and let this i be r ,
6. using a'_{is} as the pivot element, obtain the new canonical form in which α_s has replaced α_r as a unit vector.
7. Repeat the whole process until all $c'_j \geq 0$.

In many cases an immediate basic feasible solution cannot be obtained, so artificial variables ($\alpha_{n+1}, \alpha_{n+2}, \dots, \alpha_{n+k}$) must be introduced. Their removal is accomplished not by considering at first the original objective function, but by minimizing the infeasibility form W , defined by

$$W = M (\alpha_{n+1} + \alpha_{n+2} + \dots + \alpha_{n+k}) \quad (V.3)$$

where M is a large penalty coefficient.

The minimization of (V.3) is called "phase I", while the minimization of the original objective function is called "phase II". The process from one feasible solution to

another is sketched schematically in Figure 1.

The coefficient d_j can be regarded as similar to that denoted by c_j and associated with the infeasibility objective function of (V.3). When all $d_j \geq 0$ and $W = 0$, end of phase I is reached. But if W , at minimum, does not equal to zero, no feasible solution exists.

The overall procedure in solving linear programming by Simplex method is illustrated in the flow diagram of Figure 2.

In function approximation the problem is to find the minimum λ

$$\Rightarrow \left| f(x_i) - \sum_{j=0}^n \alpha_j g_j(x_i) \right| \leq \lambda \quad \text{for } 1 \leq i \leq m$$

i.e.

$$\lambda + \sum_{j=0}^n \alpha_j g_j(x_i) \geq f(x_i)$$

$$\lambda - \sum_{j=0}^n \alpha_j g_j(x_i) \geq -f(x_i)$$

With the introduction of slack and artificial variables the problem becomes

to minimize

$$Z = \lambda + M \sum_{i=1}^m u_i$$

Figure 1

Diagrammatical Representation of Simplex Method

k^{th} iteration	c_j		c_1	...	c_s	...	c_n
	Basic Vector	Values	x_1	...	x_s	...	x_n
	x_1	b'_1	a'_{11}	...	$a'_1 a'_{1s}$...	a'_{1n}
	x_2	b'_2	a'_{21}	...	$a'_2 a'_{2s}$...	a'_{2n}
	...						
	x_r	b'_r	a'_{r1}	...	a'_{rs}	...	a'_{rn}
	...						
	x_m	b'_m	a'_{m1}	...	a'_{ms}	...	a'_{mn}
	B	Z	c'_1	...	c'_s	...	c'_n
	$(-W)$	$-W_0$	d'_1	...	d'_s	...	d'_n
$k+1^{\text{st}}$ iteration	x_1	$b'_1 - a'_{1s} b^*_r$	$a'_{11} - a'_{1s} a^*_{r1}$...	0	...	$a'_{1n} - a'_{1s} a^*_{rn}$
	x_2	$b'_2 - a'_{2s} b^*_r$	$a'_{21} - a'_{2s} a^*_{r1}$...	0	...	$a'_{2n} - a'_{2s} a^*_{rn}$
	...						
	x_s	$b^*_r = b'_r / a'_{rs}$	$a^*_{r1} = a'_{r1} / a'_{rs}$...	1	...	$a^*_{rn} = a'_{rn} / a^*_{rs}$
	...						
	x_m	$b'_m - a'_{ms} b^*_r$	$a'_{m1} - a'_{ms} a^*_{r1}$...	0	...	$a'_{mn} - a'_{ms} a^*_{rn}$
	B	$Z - c_s b^*_r$	$c'_1 - c'_s a^*_{r1}$...	0	...	$c'_n - c'_s a^*_{rn}$
	$(-W)$	$-W_0 - d'_s b^*_r$	$d'_1 - d'_s a^*_{r1}$...	0	...	$d'_n - d'_s a^*_{rn}$

Figure 2

Flow Diagram for Linear Programming by
the Simplex Method.

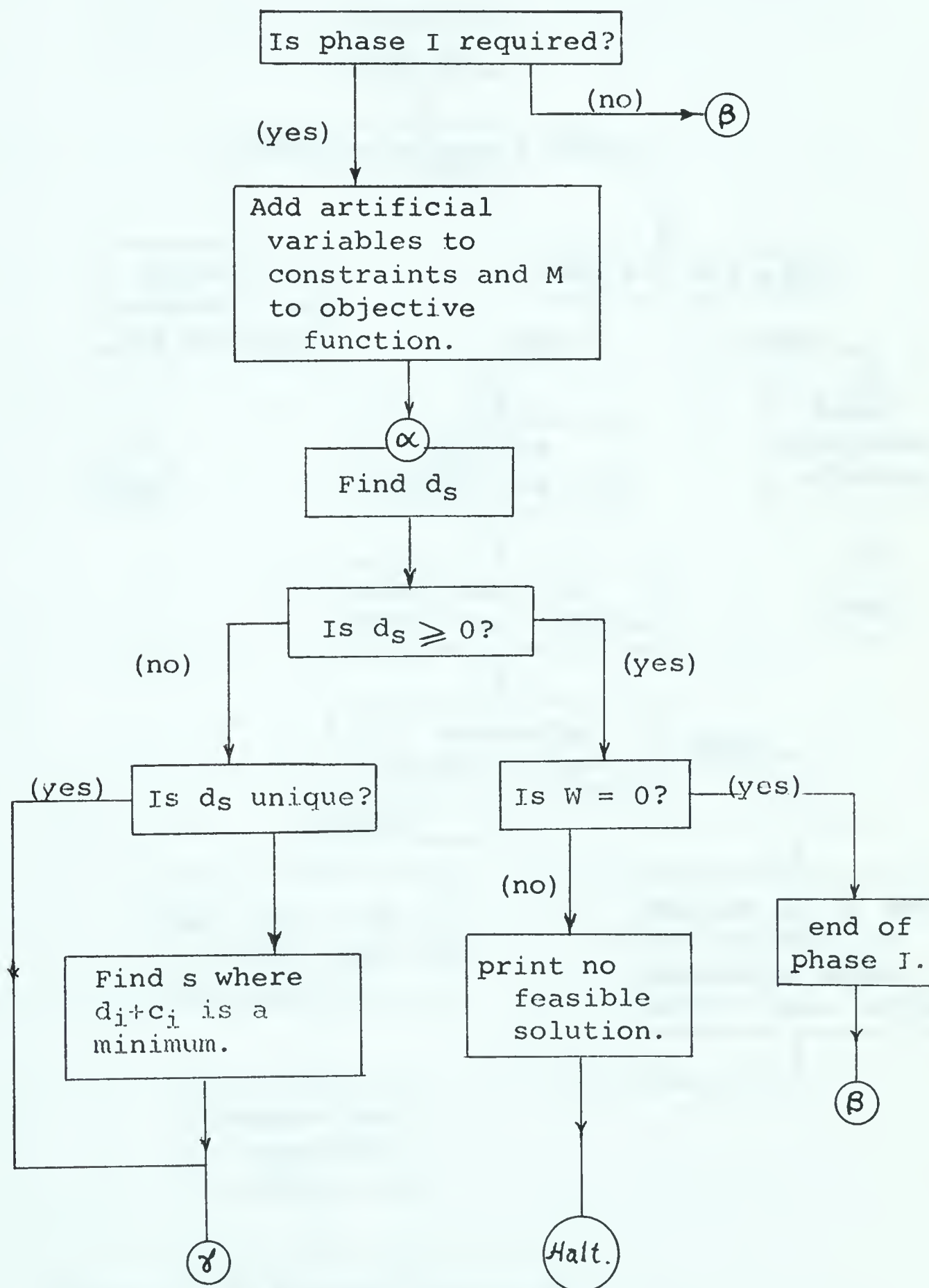
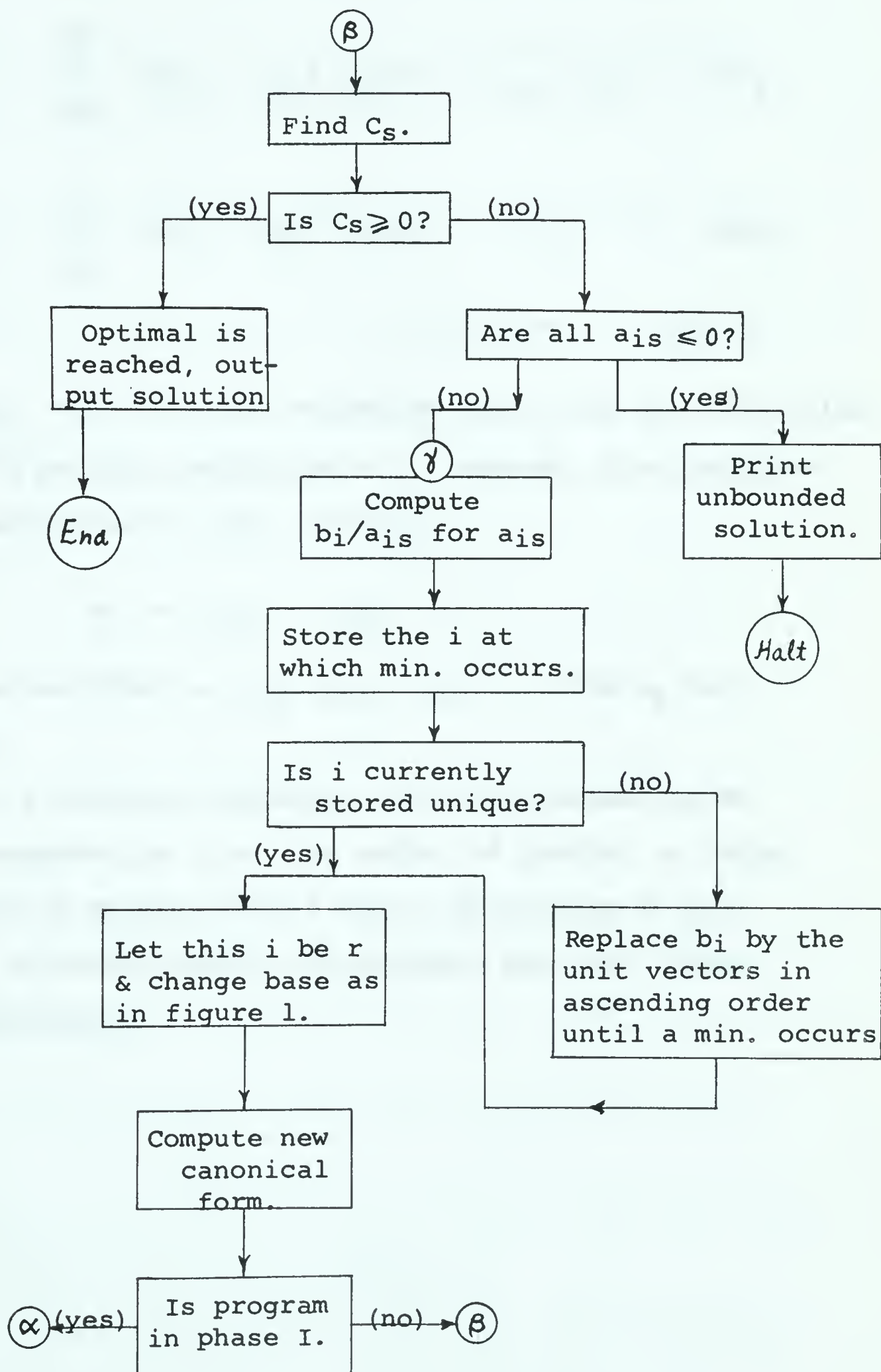


Figure 2

(continued)



subject to

$$\begin{aligned}\lambda + \sum_{j=0}^n (y_{1j} - y_{2j}) g_j(x_i) - v_{1i} + u_i &= f(x_i) \\ \lambda - \sum_{j=0}^n (y_{1j} - y_{2j}) g_j(x_i) + v_{2i} &= -f(x_i) \\ 1 \leq i \leq m &\quad (V.4)\end{aligned}$$

where v_{1i} , v_{2i} are the slack variables and u_i are the artificial variables with penalty coefficients M . However, the variables α_j are not restricted in sign, so put

$$\alpha_j = y_{1j} - y_{2j}.$$

Thus, all the variables λ , y_{1j} , y_{2j} , v_{2i} , v_i and u_i are non-negative.

It is obvious, therefore, the new problem may be too big for computation if m , the number of points, is large. An elegant way of getting around such a difficulty is proposed in the following section by applying the dual linear programming technique.

VI. FUNCTION APPROXIMATION BY DUAL LINEAR PROGRAMMING

By definition if two linear programming problems are said to be dual, they are related to one another as follows:

when the minimizing problem is considered as primal such that:

$$\text{minimize } B = c_1x_1 + c_2x_2 + \dots + c_nx_n$$

subject to

$$\sum_{j=1}^n a_{ij}x_j \geq b_i \quad (1 \leq i \leq m) \quad (\text{VI.1})$$

$$\text{with all } x_j \geq 0 \quad (1 \leq j \leq n)$$

then maximizing problem will be considered as dual such that

$$\text{maximize } Z = b_1y_1 + b_2y_2 + \dots + b_my_m$$

subject to

$$\sum_{i=1}^m a_{ji}y_i \leq c_j \quad (1 \leq j \leq n) \quad (\text{VI.2})$$

$$\text{with all } y_i \geq 0 \quad (1 \leq i \leq m).$$

The relationships between the two systems are such that:

- (i) if the objective function of one is to be minimized, then that of the other is to be maximized,
- (ii) the coefficient matrix of one system is the transpose of the other.

(iii) The constants on the right-hand side of one system are the coefficients of the objective function of the other.

As a general case consider a primal to be a mixed system consists of the following:

$$(a) \quad k \text{ constraints of type } \sum a_{ij}x_i = b_j \quad j = 1, \dots, k$$

$$(b) \quad r \text{ constraints of type } \sum a_{ij}x_i \leq b_j \quad j = k+1, \dots, k+r$$

$$(c) \quad s \text{ constraints of type } \sum a_{ij}x_i \geq b_j \quad j = k+r+1, \dots, k+r+s$$

Some of the variables are non-negative while the rest are unrestricted in sign. This primal system is the most general system possible. It is represented diagrammatically in Figure 3, with letters A, B, C, D, E and F denoting the subarrays of the coefficient matrix.

Before dualizing the primal, it is necessary to multiply the constraints $k+1, k+2, \dots, k+r$ by -1 so as to reverse the inequalities. The dual is shown schematically in the lower diagram of Figure 3, with superscript T denoting the transpose of the original subarray of the coefficient matrix.

The fundamental property which is relevant in function approximation can be stated as follows:

If X is a feasible solution vector to (VI.1) and Y a feasible solution vector to (VI.2), and

$$\sum_{j=1}^n c_j x_j = \sum_{i=1}^m b_i y_i \quad (VI.3)$$

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Figure 3

Duality of Linear Programming Problems

then X is an optimal solution vector to (VI.1) and Y is an optimal solution to (VI.2).

Now if we consider the system (IV.2) again, since α_j are not restricted in sign, the dual system with reference to Figure 3, may be written as follows:

maximize

$$\sum_{i=1}^m f_i(u_i - v_i) = Z \quad (\text{VI.4a})$$

subject to

$$\sum_{i=1}^m (u_i + v_i) \leq 1 \quad (\text{VI.4b})$$

and

$$\sum_{i=1}^m g_{ij}(u_i - v_i) = 0 \quad (\text{VI.4c})$$

for all $u_i, v_i \geq 0$ and $j = 1, 2, \dots, n$.

Now to convert the constraint (VI.4b) into an equation, a slack variable has to be introduced. However, if we assume that we are dealing with the non-trivial case, in which $\lambda > 0$, this slack variable will not enter the optimal solution at a positive level(14) - in other words this slack variable cannot be in the final basis and must therefore take a value of zero. Thus the constraint (VI.4b) can be written as

$$\sum_{i=1}^m (u_i + v_i) = 1$$

When the optimal solution is reached

$$(B)_{\text{opt.}} = (\lambda)_{\text{opt.}}$$

it can be seen that the optimal basic vector of the dual system will correspond to those constraints in the primal that gives the optimum λ . After solving these constraints in the form of equalities the various coefficients α_j and λ will be determined.

The advantage of this approach is that the number of constraints in the dual is equal to the number of coefficients plus λ ; thus, it is independent of the number of data points. Furthermore, if an extra coefficient in the primal system is required, it is equivalent to an additional constraint in the dual.

As stated in equation (I.1), g_{ij} can be any known functions with any number of independent variables. Moreover, the data points can be located in any convenient or random spacing, which is, indeed, a very significant advantage over other methods of approximation involving more than one independent variable. This approach, in fact, enjoys a high degree of freedom in approximation.

VII. APPLICATION OF DUAL LINEAR PROGRAMMING TO MULTIPLE REGRESSION ANALYSIS

In order to obtain a mathematical description of the relationship between the functional value and its variables there are several ways of approaching the problem, depending on the characteristics of the observations and on the aim of the analysis. Correlation analysis and regression analysis are two of the statistical methods. The former has been discussed in the previous section while the latter is to be described briefly in the following.

The purpose of regression analysis is to obtain a best fit of a set of observations of independent and dependent variables by an equation of the form

$$y = \sum_{i=0}^n b_i f_i (x_1, x_2, \dots, x_m)$$

where y is the dependent variable, x_1, x_2, \dots are the independent variables in some given functions, f_i and b_i are the coefficient to be determined. However it is not known whether all the independent variables x_i and the given functions f_i will provide any significant contribution to the approximation. It is the purpose of the analysis to test their significance. The criterion for accepting f_i to be an approximant is the extent of improvement in the variance upon the inclusion of f_i into the approximating equation. Hence, in the

course of analysis if an independent variable x_i or a given function f_i is tested, a least square analysis is performed and the variance is calculated. Obviously for multiple regression this method is very time consuming.

A stepwise procedure has been proposed(9), which introduces a variable or a given function at a time. However, a least square analysis must be used in obtaining the coefficients before the variance can be determined.

If the Chebyshev criterion and not the variance is to be used as a criterion for rejecting the variables or given functions and for the goodness of fit, then dual linear programming can be used in the analysis. Here we determine whether or not there is a significant change in the maximum absolute deviation.

As seen from the preceding section, with an introduction of an approximating function f_i , an extra expansion coefficient, b_i is to be determined, which is equivalent to an addition of a constraint in the dual problem. Corresponding to each additional constraint to the system, an optimum objective function $(B)_{opt.}$ can be obtained which is the maximum absolute deviation of the system. Hence, to see the significance of a certain approximating function f_i it is necessary only to compare the values of the objective function before and after the inclusion of f_i without actually solving for all the coefficients. If the value of ^{the} objective function is improved

then f_i does belong to the group. If there is no improvement on the other hand, the function f_i is to be rejected. At the end of the analysis only the functions that are of significance will remain. At this stage, we proceed as in correlation analysis and the coefficients can be evaluated accordingly.

VIII. NUMERICAL ILLUSTRATIONS

A. Curve Fitting

In order to compare the various methods we chose to use the data from "Data Systems and Processing Department of Shell Oil Company"(10), for which other curve fitting techniques have been applied. The methods of approximation are as follows:

1. power polynomials using least squares criterion,
2. self-generating orthogonal polynomials using least squares criterion,
3. Chebyshev polynomials using least squares criterion(10),
4. dual linear programming using Chebyshev criterion.

In using the Chebyshev polynomials $T_j(x)$ in the approximation

$$\text{i.e. } f(x) = c_0 + c_1 T_1(x) + c_2 T_2(x) + \dots + c_n T_n(x) \quad (\text{VIII.1})$$

the expansion coefficients are evaluated as follows:

$$c_0 = \frac{1}{n+1} \sum_{i=0}^n f(x_i)$$

and

$$c_j = \frac{1}{n+2} \sum_{i=0}^n f(x_i) T_j(x_i) \quad (\text{VIII.2})$$

where

$$x = \frac{\pi(i + 1/2)}{n+1} \quad \text{for } i = 0, 1, \dots, n.$$

In order to find $f(x_i)$, the given set of data has to be first normalized into the range of ± 1 . Then some interpolation formula is used to find $f(x_i)$. The authors of reference(10) used 3rd degree Lagrangian interpolation.

If the variance is used as the criterion for closeness of fit, all four methods yield comparable results. Indeed, since methods (1), (2) and (3) all use the least squares criterion they should theoretically have the same variance. However, the use of Chebyshev polynomials might be expected to show a higher variance due to the fact that an additional interpolation step is required. The significant higher variance shown by the power polynomials for the 5th degree case is due to the calculational difficulty encountered in solving the coefficient matrix D of equation (II.6), which tends to be ill-conditioned. For these reasons the use of orthogonal polynomials is to be preferred.

As expected, the results from the dual linear programming using Chebyshev criterion show a significant reduction in the minimal maximum absolute deviation as compared to those of the least squares analysis. But a somewhat higher variance is obtained.

We might also modify the least squares technique so as to approach the Chebyshev criterion, by using larger weighting factors on those points which show greater deviations. When these weighting factors were made proportional to their

TABLE 1

Comparison of Results in Curve Fitting
by Various Methods

Degree of Approximation	4th		5th	
Method of Approximation	Variance	Max. Abs. Deviation	Variance	Max. Abs. Deviation
Power Polynomial	2.5756×10^{-4}	0.0384	1.3125×10^{-4}	0.0240
Self-generat- ing Orthogonal Polynomials	2.6945×10^{-4}	0.0383	0.6831×10^{-4}	0.0182
Chebyshev Polynomials	3.0936×10^{-4}	0.383	0.8755×10^{-4}	0.0274
Dual Linear Programming	3.9436×10^{-4}	0.0233	1.1190×10^{-4}	0.0120

TABLE 2

Effect of Modification of Weighting Factors
on Maximum Absolute Deviations

Degree of Approximation	Maximum Absolution Deviations on			
	3rd	4th	5th	6th
(i)	0.1041	0.0383	0.0274	0.0183
(ii)	0.0909	0.0383	0.0182	0.0110
(iii)	0.0579	0.0266	0.0160	0.0083

where

- (i) from Chebyshev Polynomials(5)
- (ii) from self-generating orthogonal polynomials
- (iii) linear modification of weighting factors of (ii)
with range $1 \leq W_i \leq 5$

absolute deviations some reduction in the maximum absolute deviation was achieved as indicated in Table 2. However, even with continuous application of the linear modification procedure these maximum absolute deviations did not reach the true value obtained by the dual linear programming.

B. Surface Fitting

In the case of two-dimensional surface fitting the data are also obtained from "Data Systems and Processing Department of Shell Oil Company"(10), in which the authors used Chebyshev polynomials as the approximating polynomials, i.e.

$$f(x, y) = \sum_{i=0}^n \sum_{j=0}^m c_{ij} T_i(x) T_j(y) \quad (\text{VIII.3})$$

where the expansion coefficients are evaluated as follows:

$$c_{ij} = \frac{4}{(n+1)(m+1)} \sum_{a=0}^n T_i(x_a) \sum_{b=0}^m T_j(y_b) f(x_a, y_b) \quad (\text{VIII.4})$$

but

$$c_{00} = c_{00}/4$$

$$\text{and} \quad c_{ij} = c_{ij}/2 \quad \text{for } i = 0 \neq j \quad \text{or } j = 0 \neq i$$

with

$$x_a = \frac{\pi(a + 1/2)}{n+1}$$

$$y_b = \frac{\pi(b + 1/2)}{m+1}.$$

Again $f(x_a, y_b)$ were obtained from the given data by 3rd degree Lagrangian interpolation.

The results of surface fitting with a 4th by 4th degree polynomial as the approximating function and using the least squares criterion, are shown in Table 3. As in the case of curve fitting the self-generating orthogonal polynomials gave better results than those by the Chebyshev polynomials. This is probably also due to the fact that the interpolation of data is not necessary for the former. The use of power polynomials for surface fitting is not practicable because of the inherent computational difficulty.

TABLE 3

Surface Fitting by Least Squares Criterion

$$f(x, y) = \sum_{i=0}^n \sum_{j=0}^m A_{ij} P_i(x) Q_j(y)$$

at $n = m = 4$

x	y	f(x, y) given	Chebyshev Polynomial	Self-Generating Orthogonal Polynomial
0.2	1.10	0.3560	0.3660	0.3583
1.2	1.1	3.1800	3.2323	3.1589
0.4	1.2	0.5900	0.5852	0.5808
1.4	1.2	2.6800	2.7043	2.7043
0.5	1.3	0.6050	0.5976	0.5952
1.5	1.3	2.2300	2.2336	2.2316
0.6	1.4	0.6000	0.6042	0.6041
1.6	1.4	1.9100	1.9391	1.9296
0.8	1.5	0.7100	0.7099	0.7048
1.8	1.5	1.800	1.7655	1.7686
1.0	1.6	0.7500	0.7627	0.7652
2.0	1.6	1.6300	1.6445	1.6300
Mean absolute deviation			0.0196	0.0125
Maximum absolute deviation			0.1339	0.0538
Maximum percentage deviation			3.95	4.20

C. Evaluation of Benedict-Webb-Rubin Equation by Dual Linear Programming

If the approximating functions have to be of some given form, then the use of self-generating or any other orthogonal polynomials as approximating functions is no longer applicable, because they contain all the combinations of powers up to $x^n y^m$. For instance, if the equation of state by Benedict-Webb-Rubin(11) is required, i.e.

$$\begin{aligned}
 P(T,d) = & RTd + B_0 RTd^2 - A_0 d^2 - c_0 d^2/T^2 \\
 & + b RTd^3 - ad^3 + a\alpha d^6 \\
 & + cd^2/T^2 \left\{ (1 + \gamma d^2) \right\} \cdot \exp(-\gamma d^2)
 \end{aligned}
 \tag{VIII.5}$$

then the coefficients to be determined are B_0 , A_0 , c , b , a , α , c and γ with P , T , d and R as the known quantities. They can be obtained by a least squares analysis with γ being assumed arbitrarily. Unfortunately with every new value of γ tried, the whole process of the analysis has to be repeated. Thus, it is very time consuming.

However, if γ is assumed, then the coefficients in equation (VIII.5) will be in linear combination and linear programming can be applied.

Thus, the problem reduces to the following:

minimize λ

subject to

$$\begin{aligned} & \lambda + B_0 R T_i d_i^2 - A d_i^2 - c_0 d_i^2 / T_i^2 \\ & + b R T_i d_i^3 - a d_i^3 + \alpha_1 d_i^6 \\ & + c e^{-\gamma d_i^2} \left\{ (1 + \gamma d_i^2) \right\} d_i^2 / T_i^2 \geq (P_i - R T_i d_i) \end{aligned}$$

$$\begin{aligned} & \lambda - B_0 R T_i d_i^2 + A d_i^2 + c_0 d_i^2 / T_i^2 \\ & - b R T_i d_i^3 + a d_i^3 - \alpha_1 d_i^6 \\ & - c e^{-\gamma d_i^2} \left\{ (1 + \gamma d_i^2) \right\} d_i^2 / T_i^2 \geq -(P_i - R T_i d_i) \end{aligned}$$

$$\text{for } 1 \leq i \leq m \quad (\text{VIII.6})$$

where

$$\alpha_1 = \alpha a$$

The dual problem will be to maximize

$$\sum_{i=1}^m (P_i - R T_i d_i) (u_i - v_i) = B$$

subject to

$$\sum_{i=1}^m (u_i + v_i) = 1$$

and

$$\sum_{i=1}^m RT_i d_i^2 (u_i - v_i) = 0$$

$$\sum_{i=1}^m -d_i^2 (u_i - v_i) = 0$$

$$\sum_{i=1}^m -d_i^2/T_i^2 (u_i - v_i) = 0$$

$$\sum_{i=1}^m RT_i d_i^3 (u_i - v_i) = 0$$

$$\sum_{i=1}^m -d_i^3 (u_i - v_i) = 0$$

$$\sum_{i=1}^m d_i^6 (u_i - v_i) = 0$$

$$\sum_{i=1}^m e^{-\gamma d_i^2} (1 + \gamma d_i^2) \frac{d_i^2}{T_i} (u_i - v_i) = 0 \quad (\text{VIII.7})$$

It can be seen from the dual problem of (VIII.7) that each constraint is equivalent to an unknown in the primal. Hence, a system of $2m$ inequality equations of (VIII.6) with eight unknowns is reduced to an equivalent underdetermined

system of $2m$ unknowns and eight equations. Now with every γ tested, only the eighth constraint in equation (VIII.7) is changed and the whole system does not require repeated calculation. Hence, a series of values of γ could be tested until the optimum B is obtained.

Having obtained the optimum base of the dual problem, there arises the necessity of finding the equivalent optimum base of the primal which consists of the equations represented by the basic u_i and v_i . This system is then solved by the $L - U$ matrix inversion which is further improved by the method suggested by Hotelling(12).

The data for the approximation are taken from Douslin et al(13) and the results are tabulated in Table 4. Both least squares analysis and the dual linear programming technique were applied on the same set of data. Fortunately, the least squares technique was feasible, since the matrix resulting from the normal equation (II.6) was well-conditioned. However, even here, the linear programming technique took significantly less computer time. One of the main advantages of the dual linear programming method is its ability to handle any given functions of multi-independent variables with data randomly spaced. Furthermore, for each additional approximating function introduced into the analysis, it yields a corresponding optimum B , which reveals

TABLE 4B-W-R Equation by Various Methods

Coefficients	B-W-R (11)	Linear Programming	Least Square
B_o	0.454625×10^{-1}	$0.40905353 \times 10^{-1}$	$0.43615278 \times 10^{-1}$
A_o	1.79894	1.5725351	1.7379948
c_o	0.318382×10^5	0.4350818×10^5	0.34284477×10^5
b	0.252033×10^{-2}	$0.28653194 \times 10^{-2}$	$0.25722946 \times 10^{-2}$
a	0.435200×10^{-1}	$0.61719941 \times 10^{-1}$	$0.41383982 \times 10^{-1}$
$a\alpha$	0.143616×10^{-4}	$0.16265777 \times 10^{-4}$	$0.13092259 \times 10^{-4}$
c	0.358786×10^4	0.47144865×10^4	0.34590712×10^4
γ	0.0105000	0.0100	0.0100
Maximum Absolute Deviation	4.25 atm	0.263 atm	0.529 atm.
Maximum % Deviation	1.23	0.354	0.211

Maximum absolute deviation and maximum % deviation do not necessarily occur at the same point.

the information whether the approximation is within the allowable accuracy or further terms are required, without actual calculation of all the expansion coefficients.

D. Application of Dual Linear Programming to Multiple Regression Analysis

Assume that we want to find an approximating function $f(x,y)$ to fit a set of points (x,y) which, in fact, is generated arbitrarily from the following expression

$$F(x,y) = 3.2 + 0.7x - 3.0y + 1.4xy \quad (\text{VIII.8})$$

with $2 \leq x \leq 3$ and $1 \leq y \leq 2$.

Now suppose the approximating function to be tested is

$$f(x,y) = \alpha_1 + \alpha_2 x + \alpha_3 xy + \alpha_4 e^{-x} + \alpha_5 / y + \alpha_6 y \quad (\text{VIII.9})$$

where α_i are the expansion coefficients to be determined.

Accordingly the dual problem is to maximize

$$\sum_{i=1}^m f(x_i y_i) \cdot (u_i - v_i) = B$$

subject to

$$\sum_{i=1}^m (u_i + v_i) = 1 \quad (\text{VIII.10})$$

and

$$\sum_{i=1}^m g_{ij} \cdot (u_i - v_i) = 0 \quad \text{for } 1 \leq j \leq 6$$

where g_{ij} represent the approximating functions in (VIII.9).

The results of the analysis are shown in Table 5, so that the final approximating equation is

$$f(x,y) = \alpha_1 + \alpha_2 x + \alpha_3 xy + \alpha_5/y + \alpha_6 y$$

From the final optimum base of the dual problem the coefficients can be obtained from the corresponding equations in the primal problem to be

$$f(x,y) = 3.20 + 0.70x + 1.40xy + 0.884 \times 10^{-6}/y - 3.00y$$

exactly as in (VIII.8) if the term $(0.884 \times 10^{-6}/y)$ is neglected

The analysis was done with 36 data points in 6 seconds in IBM 7040. The advantage of this approach over the existing methods is that a direct test on a presumed approximating function can be made, by-passing each time the evaluation of coefficients and the calculation of variance until the final regressional form is obtained. Furthermore, with the addition of a new constraint, i.e. an introduction of an extra approximating function, complete analysis is not required for the evaluation of the objective function. Thus, in large systems the advantage of this method may be very significant.

TABLE 5Regression Analysis

Constraint Tested	Corresponding Function	Optimum B	Remark
g_{i0}	λ	7.70	
g_{i1}	1	1.75	accepted
g_{i2}	x	0.600	accepted
g_{i3}	xy	0.300	accepted
g_{i4}	$1/e^{\alpha}$	0.300	rejected
g_{i5}	$1/y$	0.212	accepted
g_{i6}	y	1×10^{-7}	accepted

CONCLUSION

1. If the criterion of least squares is to be used and the approximating function is to be a complete set of power polynomials, then the method of self-generating orthogonal polynomials is recommended. This method, presented in the literature for functions with one independent variable, has been extended in this work to functions with two independent variables. Since data are usually given in the form of rectangular grid, i.e. in tabular form, the developed method can always be applied directly, while the use of any other orthogonal polynomials may require an additional procedure involving data interpolation.

2. If the absolute minimal maximum deviation or Chebyshev criterion is to be used, then the method of dual linear programming is feasible and computationally efficient. The method has been successfully applied to cases with one or two independent variables. Furthermore, the approximating function can be any linear combination of specified functions and the analysis can be applied to any randomly spaced data.

3. Preliminary work indicates that the above methods give good fit for the functional values, but this does not ensure that their derivatives, obtained from the approximating functions, will yield equally reliable results. However, the linear programming techniques permit the inclusion of additional constraints with respect to the derivatives. For instance,

constraints of the form

$$\left| f'(x_i) - \sum_{j=0}^n \alpha_j g_j'(x_i) \right| \leq \lambda_1$$

can be readily included in the primal problem. Further study on this subject is recommended.

4. Due to its computational efficiency the dual linear programming technique may offer some calculational advantages over the least squares technique in conventional regression analysis. However, only preliminary work in this area has been done in this thesis and hence further study will be required.

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APPENDIX A

Derivation and Proof of the Orthogonality of Recurrence Equation (II.12)

Define the orthogonal polynomials as follows

$$P_0(x) = 1 \quad (1_0)$$

$$P_1(x) = x P_0(x) - \alpha_1 P_0(x) \quad (1_1)$$

$$P_2(x) = x P_1(x) - \alpha_2 P_1(x) - \beta_2 P_0(x) \quad (1_2)$$

$$\dots \quad \dots$$

$$P_i(x) = x P_{i-1}(x) - \alpha_i P_{i-1}(x) - \beta_i P_{i-2}(x) \quad (1_i)$$

Here the α_i and β_i are numbers constructed to make the orthogonality relationship, as follows, hold

$$\sum_{k=1}^m P_i(x_k) P_j(x_k) = 0 \quad (2)$$

for $i \neq j$. Such polynomials are said to be orthogonal over the point set (x_1, x_2, \dots, x_m) . It is proved by induction that this is indeed true.

Proof:

To find α_1 there is the equation

$$\sum_{k=1}^m P_1(x_k) P_0(x_k) = 0 \quad (3)$$

To determine α_2 and β_2 two equations are available
i.e.

$$\sum_{k=1}^m P_2(x_k) P_0(x_k) = 0 \quad (4a)$$

and

$$\sum_{k=1}^m P_2(x_k) P_1(x_k) = 0 \quad (4b)$$

Now P_0 , P_1 , P_2 by construction are mutually orthogonal to one another, i.e. satisfying (2).

Consider $P_3(x)$ as the first case in the induction,

$$P_3(x) = x P_2(x) - \alpha_3 P_2(x) - \beta_3 P_1(x) \quad (5)$$

Multiply (5) by $P_j(x_k)$ and summing over k yields

$$\begin{aligned} \sum_{k=1}^m P_3(x_k) P_j(x_k) &= \sum_{k=1}^m x_k P_2(x_k) P_j(x_k) \\ &- \alpha_3 \sum_{k=1}^m P_2(x_k) P_j(x_k) - \beta_3 \sum_{k=1}^m P_1(x_k) P_j(x_k) \end{aligned} \quad (6)$$

For $j < 3 - 2$ (i.e. $j = 0$), the last two terms in (b) are zero by (4).

Since $x P_j(x)$ is a polynomial of degree $j+1$ (i.e. 1st) in x , it can be expressed as a linear combination of ^{the} polynomials $P_0(x)$ & $P_1(x)$. Thus,

$$\sum_{k=1}^m P_2(x_k) \{ x_k P_j(x_k) \} = 0 \quad (\text{as } j = 0) \quad (7)$$

Hence $P_3(x)$ is orthogonal to $P_0(x)$ for any choices of α_3 and β_3 .

If $j = 2$, take

$$\alpha_3 = \frac{\sum_{k=1}^m x_k P_2^2(x_k)}{\sum_{k=1}^m P_2^2(x_k)} \quad (8)$$

then

$$\sum_{k=1}^m P_3(x_k) P_2(x_k) = 0. \quad (9)$$

If $j = 1$, take

$$\beta_3 = \frac{\sum_{k=1}^m x_k P_2(x_k) P_1(x_k)}{\sum_{k=1}^m P_1^2(x_k)} \quad (10)$$

then

$$\sum_{k=1}^m P_3(x_k) P_1(x_k) = 0, \quad (11)$$

Thus, P_3, P_2, P_1, P_0 are orthogonal to one another.

Now assuming $P_0(x), \dots, P_i(x)$ are mutually orthogonal with $\alpha_1, \dots, \alpha_i$ and β_2, \dots, β_i constructed to satisfy the relationship (2), it is required to determine $P_{i+1}(x)$.

Again multiplying $P_{i+1}(x_k)$ by $P_j(x_k)$ and summing over k , we get

$$\begin{aligned} \sum_{k=1}^m P_{i+1}(x_k) P_j(x_k) &= \sum_{k=1}^m P_i(x_k) \left\{ x_k P_j(x_k) \right\} \\ &- \alpha_{i+1} \sum_{k=1}^m P_i(x_k) P_j(x_k) - \beta_{i+1} \sum_{k=1}^m P_{i-1}(x_k) P_j(x_k) \end{aligned} \quad (12)$$

For $j < i - 1$ (i.e. $j = 0, 1, \dots, i-2$), the last two terms in (12) are zero. Also $x \cdot P_j(x)$ can be expressed as a linear combination of $P_0(x), \dots, P_{j+1}(x)$ (which is still lower than $P_i(x)$). Thus,

$$\sum_{k=1}^m P_i(x_k) \left\{ x_k P_j(x_k) \right\} = 0 \quad (13)$$

Taking $j = i$, and

$$\alpha_{i+1} = \frac{\sum_{k=1}^m x_k P_i^2(x_k)}{\sum_{k=1}^m P_i^2(x_k)} \quad (14)$$

then

$$\sum_{k=1}^m P_{i+1}(x_k) P_i(x_k) = 0 \quad (15)$$

In taking $j = i - 1$ and

$$\beta_{i+1} = \frac{\sum_{k=1}^m x_k P_i(x_k) P_{i-1}(x_k)}{\sum_{k=1}^m P_{i-1}^2(x_k)} \quad (16)$$

then

$$\sum_{k=1}^m P_{i+1}(x_k) P_{i-1}(x_k) = 0 \quad (17)$$

Consequently $P_{i+1}(x)$ is orthogonal to $P_0(x), \dots, P_i(x)$ if α_{i+1} and β_{i+1} are constructed as (14) and (16) respectively. This completes the proof.

APPENDIX B

Construction of Orthogonal Polynomials
of $P_i(x) \cdot Q_j(y)$

If the coefficients α_i , β_i , γ_j and δ_j are constructed by equations (III.10) and the polynomials $P_i(x)$ and $Q_j(y)$ are defined by equations (III.2) and (III.3) respectively, then the polynomial products $P_i(x) \cdot Q_j(y)$ will satisfy the orthogonality relationship (III.8)

Proof:

From equation (III.8) let

$$\emptyset = \sum_{k=1}^u \sum_{l=1}^v P_i(x_k) P_s(x_k) Q_j(y_l) Q_t(y_l) \quad (1)$$

Case 1:

$t = j$ but $s \neq i$, expanding $P_i(x_k)$ it yields

$$\begin{aligned} \emptyset = \sum_{l=1}^v Q_t^2(y_l) \sum_{k=1}^u \left\{ x_k P_{i-1}(x_k) \cdot P_s(x_k) \right. \\ \left. - \alpha_i P_{i-1}(x_k) P_s(x_k) - \beta_i P_{i-2}(x_k) \cdot P_s(x_k) \right\} \quad (2) \end{aligned}$$

It has been proved in Appendix A, if $s < i - 2$, $\emptyset \equiv 0$.

With $s = i - 1$ and

$$\alpha_i = \frac{\sum_{k=1}^u x_k P_{i-1}^2(x_k)}{\sum_{k=1}^u P_{i-1}^2(x_k)} \quad (3)$$

the second summation is zero.

Therefore,

$$\emptyset = 0.$$

With $s = i - 2$ and

$$\beta_i = \frac{\sum_{k=1}^u x_k P_{i-1}(x_k) P_{i-2}(x_k)}{\sum_{k=1}^u P_{i-2}^2(x_k)} \quad (4)$$

the second summation remains zero, so

$$\emptyset = 0.$$

Case 2:

If $s = i$, but $t \neq j$, then by similar analysis to Case 1, it can readily be shown that with

$$\gamma_j = \frac{\sum_{k=1}^v y_1 Q_{j-1}^2(y_1)}{\sum_{l=1}^v Q_{j-1}^2(y_1)} \quad (5)$$

and

$$\delta_j = \frac{\sum_{l=1}^v y_1 Q_{j-1}^2(y_1) Q_{j-2}(y_1)}{\sum_{l=1}^v Q_{j-2}^2(y_1)} \quad (6)$$

then

$$\emptyset = 0 \quad \text{for } j \neq t.$$

Thus, relationship (III.8) is proved.

APPENDIX CListings of Computer Programs and Sample Output

1. Curve Fitting with Least Squares Criterion
 - using self-generating orthogonal polynomials
2. Curve Fitting with Least Squares Criterion
 - using power polynomials
3. Curve Fitting with Chebyshev Criterion
 - using linear programming
4. Surface Fitting with Least Squares Criterion
 - using self-generating orthogonal polynomials
5. Evaluation of Benedict-Webb-Rubin Equation of State by Linear Programming
6. Evaluation of Benedict-Webb-Rubin Equation of State by Least Squares Analysis
7. Multiple Regression Analysis by Linear Programming


```

1  S1=0.0
2  S2=0.0
3  S3=0.0
4  S4=0.0
5  DO 10 K=1,M
6  S1=S1+X(K)*P(I-1,K)*X/
7  S2=S2+P(I-1,K)**2/
8  S3=S3+X(K)*P(I-1,K)*P(I-2,K)
9  S4=S4+P(I-2,K)**2/
10  AX(I)=S1/S2
11  BX(I)=S3/S4
12  WRITE (6,21) AX(I), BX(I)
13  FORMAT (1H, 2(4X, F10.4))
14  DO 20 K=1,M
15  P(I,K)=(X(K)-AX(I))*P(I-1,K)-BX(I)*P(I-2,K)
16  C(1)=0.0
17  C(2)=0.0
18  DO 24 K=1,M
19  C1=C1+Y(K)*P(J,K)
20  C2=C2+P(J,K)**2/
21  C(I)=C1/C2
22  WRITE (6,25) J, C(I)
23  FORMAT (1H, 4X, I2, 3X, F10.4)
24  CHECK THE APPROXIMATION.
25  WRITE (6,26)
26  FORMAT (1H, 6X, 10X, 9X, 1H, 5X, F10.4, 7, 1X, F10.4,
27  DO 30 I=1,M
28  W=0.0
29  DO 31 J=1,NA
30  W=W+(C(J)*P(J,I))
31  D=ABS(W-Y(I))
32  WRITE (6,32) X(I), Y(I), W, D
33  FORMAT (1H, 3X, F6.2, 3X, F6.2, 3X, F6.4, 4X, F6.4)
34  CONVERSION OF ORTHOGONAL TO POLAR POLYNOMIALS.
35  P(1,1)=1.00
36  P(2,2)=1.00
37  P(2,1)=-AX(1)
38  P(3,3)=1.00
39  P(3,2)=P(2,1)-AX(2)*P(2,2)
40  P(3,1)=-P(2,1)*AX(2)-BX(2)
41  DO 40 I=4,NA
42  IA=I-1
43  JA=I-2
44  P(I,I)=P(IA,IA)
45  P(I,IA)=P(IA,JA)-AX(IA)*P(IA,I)
46  DO 41 J=2,JA
47  JB=I-J
48  P(I,JB)=P(IA,JB-1)-BX(IA)*P(IA,JB)-AX(IA)*P(IA,JB-1)
49  P(I,1)=-AX(IA)*P(IA,1)-BX(IA)*P(IA,JB)

```


20.00 4.4770
21.00 4.5826
22.00 4.6884
23.00 4.7954
24.00 4.9043
25.00 5.0150
4
1
5
-1

(EXAMPLE CONT'D.)

DEGREE OF APPROXIMATION = 5

COEFFICIENTS OF ORTHOGONAL POLYNOMIALS.
A_λ(i) B_λ(i)

0.13000000E+02 0.
0.13000000E+02 0.52500000E+02
0.12100000E+02 0.41400000E+02
0.13000000E+02 0.39600000E+02
0.12000000E+02 0.38866667E+02

T
1 0.3425355E+01
2 0.6814777E+01
3 -0.3829008E+02
4 0.7107632E+02
5 -0.1446514E+04
6 0.1110164E+06

X	Y	ΔL = Y -	10 ⁶ W
1.00	1.00	1.0000	0.0000
2.00	1.41	0.3950	0.0083
3.00	1.74	0.7200	0.0121
4.00	2.00	0.9991	0.0130
5.00	2.24	0.7425	0.0167
6.00	2.43	0.4788	0.0094
7.00	2.65	0.5337	0.0071
8.00	2.83	0.5335	0.0040
9.00	3.00	0.0000	0.0000
10.00	3.16	0.1580	0.0034
11.00	3.32	0.3109	0.0078
12.00	3.46	0.4576	0.0169
13.00	3.61	0.6000	0.0086
14.00	3.74	0.7382	0.0004
15.00	3.87	0.8720	0.0000
16.00	4.00	0.0000	0.0000

17.00	4.12	4.1400	0.0048
18.00	4.24	4.2483	0.0057
19.00	4.36	4.3567	0.0060
20.00	4.47	4.4748	0.0027
21.00	4.58	4.5817	0.0003
22.00	4.69	4.6883	0.0046
23.00	4.80	4.7944	0.0064
24.00	4.90	4.8950	0.0041
25.00	5.00	5.0067	0.0067

FINAL COEFFICIENTS OF THE POWER POLYNOMIAL.

I	A(I)
1	0.56622618E+00
2	0.48824642E-00
3	-0.41823675E-01
4	0.25467160E-02
5	-0.86586718E-04
6	0.11101640E-05

X	Y	YAL	DEV
1.00	1.00	1.0189	0.0189
2.00	1.41	1.3080	0.1080
3.00	1.73	1.7200	0.0121
4.00	2.00	1.9491	0.0009
5.00	2.24	2.2428	0.0057
6.00	2.45	2.4889	0.0064
7.00	2.65	2.6530	0.0078
8.00	2.83	2.8330	0.0046
9.00	2.98	2.9533	0.0003
10.00	3.16	3.1580	0.0034
11.00	3.32	3.3559	0.0058
12.00	3.46	3.4576	0.0067
13.00	3.61	3.6000	0.0086
14.00	3.74	3.7383	0.0034
15.00	3.87	3.8725	0.0009
16.00	4.00	4.1025	0.0025
17.00	4.12	4.1279	0.0048
18.00	4.24	4.2483	0.0057
19.00	4.36	4.3584	0.0091
20.00	4.47	4.4748	0.0027
21.00	4.58	4.5817	0.0003
22.00	4.69	4.6883	0.0046
23.00	4.80	4.7944	0.0064
24.00	4.90	4.8950	0.0040
25.00	5.00	5.0067	0.0067

VARIANCE = 0.68548621E-04

LEAST SQUARE ANALYSIS OF THE POWER POLYNOMIAL IS AN APPROXIMATING FUNCTION.
THE ANALYSIS IS DONE BY THE LEAST SQUARE METHOD.
THE COEFFICIENTS OF THE APPROXIMATING FUNCTION ARE GIVEN UNDER FINAL SOLUTIONS.

(SAMPLE OUTPUT)

LEAST SQUARE ANALYSIS - POWER POLYNOMIAL.

DEGREE OF APPROXIMATION = 5

FINAL SOLUTIONS.

0.56745695E+00
0.48783131E-02
-0.41742623E-03
0.26392626E-02
-0.86172877E-04
0.11031234E-05

X	Y	Y - Y ₀	(Y - Y ₀) ²
1.0000	0.10160040E+01	0.10160040E+01	0.10322560E+02
2.0000	0.14142000E+01	0.13959147E+01	0.19485914E+02
3.0000	0.17321000E+01	0.17108154E+01	0.29268954E+02
4.0000	0.20000000E+01	0.19788824E+01	0.39160000E+02
5.0000	0.22351000E+01	0.22477440E+01	0.50333000E+02
6.0000	0.24495000E+01	0.24388300E+01	0.59500000E+02
7.0000	0.26458000E+01	0.26330880E+01	0.69330000E+02
8.0000	0.28284000E+01	0.28337600E+01	0.80150000E+02
9.0000	0.30000000E+01	0.30375660E+01	0.92250000E+02
10.0000	0.31622000E+01	0.31583430E+01	0.99750000E+02
11.0000	0.33166000E+01	0.32116040E+01	0.10395000E+03
12.0000	0.34641000E+01	0.34187824E+01	0.11689000E+03
13.0000	0.36056000E+01	0.36316800E+01	0.13180000E+03
14.0000	0.37417000E+01	0.37415460E+01	0.13990000E+03
15.0000	0.38730000E+01	0.38358020E+01	0.14685000E+03
16.0000	0.40000000E+01	0.40067620E+01	0.16055000E+03
17.0000	0.41231000E+01	0.41173000E+01	0.17040000E+03
18.0000	0.42426000E+01	0.42543330E+01	0.18090000E+03
19.0000	0.43589000E+01	0.43111840E+01	0.18680000E+03
20.0000	0.44721000E+01	0.44824606E+01	0.20080000E+03
21.0000	0.45826000E+01	0.45618000E+01	0.20700000E+03
22.0000	0.46914000E+01	0.46937600E+01	0.21830000E+03
23.0000	0.47989000E+01	0.48000140E+01	0.22840000E+03
24.0000	0.49050000E+01	0.49103480E+01	0.23850000E+03
25.0000	0.50000000E+01	0.50123988E+01	0.24840000E+03

VARIANCE = 0.13125054E-03

CURVE FITTING BY CHEBYSHEV CRITERION USING POWER POLYNOMIALS.

PART I - LINEAR PROGRAMMING BY SIMPLEX METHOD.
FOR EACH POWER TERM INTRODUCED AN OPTIMAL VALUE AND A
CORRESPONDING COEFFICIENT GIVEN.

(EXAMPLE OUTPUT)

THOUGH CHEBYSHEV APPROXIMATION BY SQUARE ERROR METHOD.

OBJECTIVE VALUE = $0.20000000E+00$
INDEP. VECTOR 25 $0.00000000E+00$
INDEP. VECTOR 26 $0.00000000E+00$

OPTIMAL VALUE = $0.2222222E-01$
INDEP. VECTOR 5 $0.00000000E+00$
INDEP. VECTOR 26 $0.00000000E+00$
INDEP. VECTOR 5 $0.00000000E+00$
\$ \$ \$ \$ \$

OPTIMAL VALUE = $0.11442584E-01$
INDEP. VECTOR 4 $0.41582442E+00$
INDEP. VECTOR 26 $0.2734444E+00$
INDEP. VECTOR 42 $0.2747546E+00$
INDEP. VECTOR 25 $0.8447556E+00$
\$ \$ \$ \$ \$

OPTIMAL VALUE = $0.4935872E-01$
INDEP. VECTOR 2 $0.00000000E+00$
INDEP. VECTOR 26 $0.00000000E+00$
INDEP. VECTOR 35 $0.00000000E+00$
INDEP. VECTOR 25 $0.127416E+00$
INDEP. VECTOR 25 $0.4947444E+00$
\$ \$ \$ \$ \$

OPTIMAL VALUE = $0.2526161E-01$
INDEP. VECTOR 2 $0.3587634E+00$
INDEP. VECTOR 26 $0.2533783E+00$
INDEP. VECTOR 32 $0.1688405E+00$
INDEP. VECTOR 15 $0.1572494E+00$
INDEP. VECTOR 47 $0.8188187E+00$
INDEP. VECTOR 25 $0.2508706E+00$
\$ \$ \$ \$ \$

PART II - SECTION OF FINAL POLYNOMIAL - 17.18.1000.1
 THE EXHIBITION OF THE FIRST AND SECOND ORDER POLYNOMIALS
 WITH THE FIRST ORDER OF THE MINIMAL POLYNOMIAL
 DEVIATION FOR THE EXHIBITION.

PROBLEM - EFFICIENT FOR FIRST POLYNOMIAL DEVIATION - 17.18.1000.1.

FINAL SOLUTIONS.

0.23461672E-11
 0.60387616E+00
 0.44765074E-00
 -0.29417882E-01
 0.32227758E-02
 -0.19312127E-04

X	F(X)	VAL.	DEF.
1.00	1.0000	1.0233	0.0033
2.00	1.4142	1.3464	0.0282
3.00	1.7321	1.6734	0.0415
4.00	2.0000	1.9971	0.0029
5.00	2.2361	2.2477	0.0114
6.00	2.4495	2.4078	0.0414
7.00	2.6458	2.6571	0.0113
8.00	2.8284	2.8474	0.0186
9.00	3.0000	3.0141	0.0141
10.00	3.1623	3.1611	0.0012
11.00	3.3166	3.3135	0.0031
12.00	3.4641	3.4674	0.0033
13.00	3.6056	3.6079	0.0023
14.00	3.7417	3.7472	0.0055
15.00	3.8730	3.8497	0.0233
16.00	4.0000	4.0013	0.0013
17.00	4.1231	4.1041	0.0190
18.00	4.2426	4.2857	0.0431
19.00	4.3589	4.3818	0.0229
20.00	4.4721	4.4840	0.0119
21.00	4.5826	4.6326	0.0490
22.00	4.6896	4.7137	0.0241
23.00	4.7930	4.8100	0.0170
24.00	4.8930	4.9041	0.0111
25.00	5.0000	4.9949	0.0051

VARIANCE = 0.40419881E-01

* * * *

1. 700
2. 800
3. 900
4. 1000
5. 1100
6. 1200
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35

[illegible]

(SAMPLE COLLECTION)

HEIGHT OF APPROXIMATION = 4 A 4

EXPANSION OF $\lambda(\lambda+1) = 10\sqrt{5}$.

1	0	$0.152470000 + 0.1$
1	1	$-0.152470000 + 0.1$
1	2	$-0.152470000 + 0.1$
1	3	$0.152470000 + 0.1$
1	4	$-0.152470000 + 0.1$
1	5	$0.152470000 + 0.1$
1	6	$-0.152470000 + 0.1$
1	7	$0.152470000 + 0.1$
1	8	$-0.152470000 + 0.1$
1	9	$0.152470000 + 0.1$
1	10	$-0.152470000 + 0.1$
1	11	$0.152470000 + 0.1$
1	12	$-0.152470000 + 0.1$
1	13	$0.152470000 + 0.1$
1	14	$-0.152470000 + 0.1$
1	15	$0.152470000 + 0.1$
1	16	$-0.152470000 + 0.1$
1	17	$0.152470000 + 0.1$
1	18	$-0.152470000 + 0.1$
1	19	$0.152470000 + 0.1$
1	20	$-0.152470000 + 0.1$
1	21	$0.152470000 + 0.1$
1	22	$-0.152470000 + 0.1$
1	23	$0.152470000 + 0.1$
1	24	$-0.152470000 + 0.1$
1	25	$0.152470000 + 0.1$
1	26	$-0.152470000 + 0.1$
1	27	$0.152470000 + 0.1$
1	28	$-0.152470000 + 0.1$
1	29	$0.152470000 + 0.1$
1	30	$-0.152470000 + 0.1$
1	31	$0.152470000 + 0.1$
1	32	$-0.152470000 + 0.1$
1	33	$0.152470000 + 0.1$
1	34	$-0.152470000 + 0.1$
1	35	$0.152470000 + 0.1$
1	36	$-0.152470000 + 0.1$
1	37	$0.152470000 + 0.1$
1	38	$-0.152470000 + 0.1$
1	39	$0.152470000 + 0.1$
1	40	$-0.152470000 + 0.1$
1	41	$0.152470000 + 0.1$
1	42	$-0.152470000 + 0.1$
1	43	$0.152470000 + 0.1$
1	44	$-0.152470000 + 0.1$
1	45	$0.152470000 + 0.1$
1	46	$-0.152470000 + 0.1$
1	47	$0.152470000 + 0.1$
1	48	$-0.152470000 + 0.1$
1	49	$0.152470000 + 0.1$
1	50	$-0.152470000 + 0.1$

$\lambda(K)$	$\lambda(L)$	$\lambda(K, L)$	λ	$\lambda(K)$
0.20	1.10	0.152470000	0.152470000	0.152470000
1.20	1.10	0.152470000	0.152470000	0.152470000
0.30	1.20	0.152470000	0.152470000	0.152470000
1.30	1.20	0.152470000	0.152470000	0.152470000
0.40	1.30	0.152470000	0.152470000	0.152470000
1.40	1.30	0.152470000	0.152470000	0.152470000
0.50	1.40	0.152470000	0.152470000	0.152470000
1.50	1.40	0.152470000	0.152470000	0.152470000
0.60	1.50	0.152470000	0.152470000	0.152470000
1.60	1.50	0.152470000	0.152470000	0.152470000
0.70	1.60	0.152470000	0.152470000	0.152470000
1.70	1.60	0.152470000	0.152470000	0.152470000

COEFFICIENTS OF POWER POLYNOMIALS.

1	0	0.0000000000000000
1	1	0.0000000000000000
1	2	-0.0000000000000000
1	3	0.0000000000000000
1	4	-0.0000000000000000
1	5	0.0000000000000000
2	1	-0.0000000000000000
2	2	0.0000000000000000
2	3	-0.0000000000000000
2	4	0.0000000000000000
2	5	-0.0000000000000000
3	1	0.0000000000000000
3	2	-0.0000000000000000
3	3	0.0000000000000000
3	4	-0.0000000000000000
3	5	0.0000000000000000
4	1	-0.0000000000000000
4	2	0.0000000000000000
4	3	-0.0000000000000000
4	4	0.0000000000000000
4	5	-0.0000000000000000
5	1	0.0000000000000000
5	2	-0.0000000000000000
5	3	0.0000000000000000
5	4	-0.0000000000000000
5	5	0.0000000000000000


```

      IF (RA(J).LT.0.0) GO TO 24
25  GA=RA(J)
      JJ=J
      GO TO 26
24  CONTINUE
26  IF (JJ.GT.JA) GO TO 252
261 JC=JJ+1
      DO 27 J=JC,JA
      IF (RA(J).LT.0.0) GO TO 27
      IF (RA(J).GT.0A) GO TO 27
      IF (PA(J).EQ.04) GO TO 29
28  QA=RA(J)
      JJ=J
      GO TO 27
29  IF (K(JJ).GT.K(J)) GO TO 27
30  QA=RA(J)
      JJ=J
27  CONTINUE
262 DIV=G(JJ,IA)
      B(JJ)=B(JJ)/DIV
      DO 31 I=1,MM
31  G(JJ,I)=G(JJ,I)/DIV
      DO 32 J=1,JA
      IF (J.EQ.JJ) GO TO 32
      DJA=G(J,IA)
      B(J)=B(J)-DJA*B(JJ)
      DO 33 I=1,MM
      IF (J.EQ.1A) GO TO 36
35  G(J,I)=G(J,I)-DJA*G(JJ,I)
      GO TO 33
36  G(J,I)=0.00
33  CONTINUE
32  CONTINUE
      RB=RB-D(1A)*B(JJ)
      DO 34 I=1,MM
      IF (1.EQ.1A) GO TO 34
37  C(I)=C(I)-C(1A)*G(JJ,I)
34  CONTINUE
      C(1A)=0.00
      K(JJ)=1A
      IF (PH.GT.1.0) GO TO 192
      IF (JJ.GT.JA) GO TO 41
40  W=W-D(1A)*B(JJ)
      DO 42 I=1,MM
      IF (J.EQ.1A) GO TO 42
43  D(I)=D(I)-D(1A)*G(JJ,I)
42  CONTINUE
      D(1A)=0.00
      GO TO 191
41  PH=2.00
192  QB=C(1)
      1A=1
      DO 192 I=2,MM

```



```

      IF (O3.EF.C(1)) GO TO 192
191  QR=C(1)
      TA=1
192  CONTINUE
      IF (O4.EF.C(1)) GO TO 193
195  WRITE (6,80) RQ
80  FORMAT (1H0, 15X, 16HORDERING VALUE = , F15.8)
      WRITE (6,81) (K(J), R(J), J=1, JA)
      WRITE (6,200)
200  FORMAT (1H-, 10X, 10H- - - - -)
      IF (JA.EF.MA) GO TO 190
196  READ (5,50) GAM
50  FORMAT (1X, F12.5)
      IF (GAM.EF.W(1)) GO TO 51
      WRITE (6,54) GAM
54  FORMAT (1H0, 15X, 8HGGAMMA = , F15.8)
      IF (LA.GT.1) GO TO 305
      LA=LA+1
      QR5=QR
      DO 300 J=1,JA
      KQ(J)=K(J)
      RQ(J)=R(J)
      DO 300 I=1,MM
197  Q(J,I)=G(J,I)
      DO 301 I=1,MM
301  QC(I)=C(1)
      GO TO 52
305  JA=JA-1
      RF=Q-R
      DO 306 J=1,JA
      K(J)=KQ(J)
      R(J)=RQ(J)
      DO 306 I=1,MM
306  G(J,I)=Q(J,I)
      DO 307 I=1,MM
307  C(I)=QC(I)
52  DO 53 I=1,7
      FA=(GAM*OF(1)*OF(1))
      IF (FA.GT.50.0) FA=50.0
53  G(8,1)=(1.0+FA)*OF(1)*X/(T(1)*T(1)*AP(10))
      JA=7
      GO TO 190
51  WRITE (6,55)
55  FORMAT (1H-, 15X, 20HEND OF PART ONE ANALYSIS.)
      END

```

ENTRY PT. I

136	1		
21.2760	273.160	1.000	
40.5160	273.160	2.000	
58.0726	273.160	3.000	
74.3221	273.160	4.000	
89.6142	273.160	5.000	
104.2480	273.160	6.000	

118.7180	213.160	1.000
133.6390	213.160	2.000
144.0170	213.160	3.000
157.1870	213.160	10.000
164.3375	213.160	1.000
177.7212	213.160	2.000
187.3094	213.160	3.000
194.2618	213.160	4.000
112.1670	213.160	5.000
131.2039	213.160	6.000
150.3520	213.160	7.000
164.3300	213.160	8.000
190.9940	213.160	9.000
214.1010	213.160	10.000
23.7173	303.152	1.000
46.1416	303.152	2.000
67.0750	303.152	3.000
86.9871	303.152	4.000
106.3360	303.152	5.000
125.4970	303.152	6.000
144.8890	303.152	7.000
164.5490	303.152	8.000
186.2650	303.152	9.000
209.3260	303.152	10.000
37.4248	323.151	1.000
61.5277	323.151	2.000
84.2087	323.151	3.000
106.3700	323.151	4.000
128.3300	323.151	5.000
150.6950	323.151	6.000
173.6650	323.151	7.000
198.7140	323.151	8.000
224.3930	323.151	9.000
253.2170	323.151	10.000
27.8521	343.153	1.000
54.5053	343.153	2.000
80.3269	343.153	3.000
105.6940	343.153	4.000
131.0430	343.153	5.000
156.8180	343.153	6.000
183.4340	343.153	7.000
211.4170	343.153	8.000
241.9656	343.153	9.000
274.4120	343.153	10.000
44.6747	373.160	1.000
73.4508	373.160	2.000
101.8530	373.160	3.000
130.2870	373.160	4.000
159.2110	373.160	5.000
189.0800	373.160	6.000
220.5180	373.160	7.000
254.1610	373.160	8.000
291.5270	373.160	9.000

32.214	328.1300	18.0000
63.1312	328.1300	18.0000
44.4728	328.1300	18.0000
125.3120	328.1300	18.0000
158.2432	328.1300	18.0000
181.1588	328.1300	18.0000
235.1152	328.1300	18.0000
262.4441	328.1300	18.0000
302.2080	328.1300	18.0000
345.4310	328.1300	18.0000
51.5763	423.183	18.5000
85.2164	423.183	18.5000
114.3300	423.183	18.5000
153.7440	423.183	18.5000
180.1340	423.183	18.5000
227.1230	423.183	18.5000
266.8010	423.183	18.5000
300.4210	423.183	18.5000
345.7800	423.183	18.5000
36.5545	443.197	18.5000
12.4316	443.197	18.5000
114.3230	443.197	18.5000
146.1460	443.197	18.5000
185.1770	443.197	18.5000
225.3010	443.197	18.5000
267.6410	443.197	18.5000
313.1460	443.197	18.5000
362.4320	443.197	18.5000
58.1860	473.213	18.5000
47.1880	473.213	18.5000
136.1150	473.213	18.5000
177.5610	473.213	18.5000
220.1440	473.213	18.5000
265.1653	473.213	18.5000
312.4320	473.213	18.5000
364.6630	473.213	18.5000
43.8456	493.227	18.5000
82.1866	493.227	18.5000
123.4990	493.227	18.5000
167.1173	493.227	18.5000
212.0210	493.227	18.5000
259.1200	493.227	18.5000
310.4310	493.227	18.5000
363.4410	493.227	18.5000
64.7607	523.245	18.5000
108.1130	523.245	18.5000
154.0100	523.245	18.5000
201.0040	523.245	18.5000
250.2320	523.245	18.5000
302.6410	523.245	18.5000
358.1640	523.245	18.5000
45.2272	48.260	18.5000
91.2710	48.260	18.5000

138.4140	4.26	3.70
187.3680	48.280	4.000
238.5010	48.280	5.100
297.0010	48.26	6.100
350.2710	48.26	7.100
41.4140	48.274	8.100
121.4120	48.274	9.100
171.2740	48.274	10.100
224.2880	48.274	11.100
280.3730	48.274	12.100
340.5060	48.274	13.100
40.5510	48.285	14.100
103.3090	48.285	15.100
152.1790	48.285	16.100
201.160	48.285	17.100
255.1580	48.285	18.100
326.4370	48.285	19.100
397.8670	48.285	20.100
78.0693	62.204	21.100
122.1370	62.204	22.100
189.4430	62.204	23.100
247.5240	62.204	24.100
310.3050	62.204	25.100
377.3660	62.204	26.100
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EVALUATION OF BENEDICT-WEER-ROBIN EQUATION WITH STAT² WITH HARTLEY CRITERION.

(SAMPLE OUTPUT)

FIGURE EVALUATION OF B-W-R EQUATION -- PART 1.

GAMMA = 0.100000E+00

OPTIMAL VALUE = 1.378800E+00

INDEP. VECTOR 266	0.13324154E+00
INDEP. VECTOR 67	7.20342020E-01
INDEP. VECTOR 133	0.2292670E-01
INDEP. VECTOR 176	0.19178252E-01
INDEP. VECTOR 19	0.7240430E-01
INDEP. VECTOR 166	0.4820744E-01
INDEP. VECTOR 141	0.1432471E-01
INDEP. VECTOR 174	0.4030100E-01

GAMMA = 0.50000000E+01

OPTIMAL VALUE = 0.3483347E+00

INDEP. VECTOR	266	0.10000000E+00
INDEP. VECTOR	6	0.14185743E+00
INDEP. VECTOR	133	0.20000000E+00
INDEP. VECTOR	140	0.41041180E+01
INDEP. VECTOR	134	0.40000000E+01
INDEP. VECTOR	166	0.20320150E+00
INDEP. VECTOR	139	0.57440013E+01
INDEP. VECTOR	9	0.16751040E+00

GAMMA = 0.10000000E+01

OPTIMAL VALUE = 0.26712095E+00

INDEP. VECTOR	266	0.17647242E+00
INDEP. VECTOR	67	0.13051000E+00
INDEP. VECTOR	133	0.27478814E+00
INDEP. VECTOR	136	0.1070222E+01
INDEP. VECTOR	13	0.49017133E+01
INDEP. VECTOR	137	0.10100000E+00
INDEP. VECTOR	191	0.13583360E+00
INDEP. VECTOR	4	0.60082667E+01

GAMMA = 0.10000000E+01

OPTIMAL VALUE = 0.35807921E+00

INDEP. VECTOR	266	0.13747000E+00
INDEP. VECTOR	69	0.20032820E+00
INDEP. VECTOR	133	0.22432000E+00
INDEP. VECTOR	136	0.12071534E+00
INDEP. VECTOR	13	0.12210000E+00
INDEP. VECTOR	166	0.00000000E+00
INDEP. VECTOR	141	0.34281000E+00
INDEP. VECTOR	144	0.40000000E+00

END OF PART ONE ANALYSIS

EVALUATION OF FINAL FIVE-FOUR EQUATIONS OF STATE BY LEAST SQUARE ANALYSIS OF THE 1960 SET OF DATA AT GIVEN PRESSURES.

(SAMPLE OUTPUT)

TABLE 1 LEAST SQUARE ANALYSIS OF FIVE-FOUR EQUATION OF STATE.

FINAL SOLUTIONS.

0.43615278E+01
 0.12374248E+01
 0.34284479E+04
 0.75722946E+03
 0.41383982E+01
 0.13092259E+04
 0.34590712E+04

TEMP	DENSITY	PRESS	CAL.P.	DEV.	P.E.
273.160	1.0000	21.276	21.276	0.000	0.000
273.160	4.000	14.323	4.366	0.000	0.000
273.160	9.000	14.114	14.947	0.000	0.000
298.153	3.500	15.303	75.238	0.000	0.000
298.153	10.500	214.100	214.323	0.000	0.000
303.152	3.000	15.336	105.332	0.000	0.000
303.152	10.000	234.325	203.324	0.000	0.000
323.151	7.500	173.653	173.750	0.000	0.000
343.153	7.000	183.434	183.450	0.000	0.000
343.153	8.000	241.35	241.453	0.000	0.000
343.160	3.500	44.612	44.630	0.000	0.000
343.160	4.500	240.527	240.441	0.000	0.000
398.170	2.000	63.737	63.743	0.000	0.000
398.170	10.000	145.703	145.802	0.000	0.000
423.183	4.500	153.777	154.081	0.000	0.000
423.183	7.500	266.831	266.888	0.000	0.000
443.197	1.000	36.763	36.742	0.000	0.000
443.197	7.000	257.637	257.633	0.000	0.000
473.213	8.000	354.557	354.553	0.000	0.000
493.220	2.000	92.028	92.014	0.000	0.000
493.220	3.000	383.443	383.390	0.000	0.000
523.245	6.500	307.547	307.638	0.000	0.000
543.250	2.000	71.238	71.102	0.000	0.000
573.274	2.500	170.477	170.317	0.000	0.000
573.274	4.500	224.288	224.228	0.000	0.000
603.285	4.000	211.808	211.354	0.000	0.000
603.285	7.000	311.853	311.771	0.000	0.000
623.294	3.500	158.443	158.228	0.000	0.000
623.294	6.500	317.358	317.454	0.000	0.000


```

25 IF (PA(1).LT.0.0) GO TO 24
    OA=PA(1)
    JJ=J
    GO TO 26
24 CONTINUE
26 IF (JJ.GE.JA) GO TO 28
261 JC=JJ+1
    DO 27 J=JC,JA
        IF (PA(J).LT.0.0) GO TO 27
        IF (PA(J).GT.0.0) GO TO 27
        IF (PA(J).EQ.0.0) GO TO 24
28 OA=PA(1)
    JJ=J
    GO TO 27
29 IF (K(JJ).GE.K(J)) GO TO 27
30 OA=PA(J)
    JJ=J
27 CONTINUE
262 DIV=G(JJ,IA)
    WRITE (6,87) JJ, IA, G(JJ,IA)
87 FORMAT (1H, 13X, 14, 3X, 13, 3X, 13H, 6)
    R(JJ)=R(JJ)/DIV
    DO 31 I=1,MM
21 G(JJ,I)=G(JJ,I)/DIV
    DO 32 J=1,JA
        IF (J.EQ.JJ) GO TO 32
        DJA=G(J,IA)
        R(J)=R(J)-DJA*R(JJ)
    DO 33 I=1,MM
35 G(J,I)=G(J,I)-DJA*R(JJ,I)
    GO TO 32
36 G(J,IA)=0.0
33 CONTINUE
32 CONTINUE
    RB=RB-(IA)*R(JJ)
    DO 34 I=1,MM
        IF (I.EQ.IA) GO TO 34
27 C(I)=C(I)-(IA)*G(JJ,I)
34 CONTINUE
    C(IA)=0.0
    K(JJ)=IA
    IF (PH.GT.1.0) GO TO 102
    IF (JJ.GE.JA) GO TO 41
41 W=W-D(IA)*R(JJ)
    DO 42 I=1,MM
        IF (I.EQ.IA) GO TO 42
43 D(I)=D(I)-D(IA)*G(JJ,I)
42 CONTINUE
    D(IA)=0.0
    GO TO 101
40 PH=2.0
102 RB=R(JJ)

```

APPENDIX

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```

1A=1
DO 100 I=1,MM
IF (Q5.IE.0) GO TO 1000
1003 QH=C(I)
1A=1
1002 CONTINUE
IF (Q5.IE.0) GO TO 1003
WRITE (6,80) R
1001 FORMAT (1H, 10X, 16F8.1)
WRITE (6,81) (K(J), R(J), J=1, JA)
CHECK=QB-R
IF (CHECK.IE.0) GO TO 201
QB=R
DO 300 J=1,JA
KQ(J)=K(J)
RQ(J)=R(J)
DO 300 I=1,MM
300 Q(J,I)=G(J,I)
DO 301 I=1,MM
301 QC(I)=C(I)
JA=JA+1
WRITE (6,181)
180 FORMAT (1H, 10X, 12F8.1)
IF (KA.IE.0) GO TO 100
WRITE (6,51)
51 FORMAT (1H, 10X, 25F8.1)
GO TO 106
201 WRITE (6,181) KA
181 FORMAT (1H, 10X, 30F8.1)
WRITE (6,180)
IF (KA.GE.40) GO TO 106
R=QB
DO 305 J=1,JP
K(J)=KQ(J)
R(J)=RQ(J)
DO 306 I=1,MM
306 G(J,I)=Q(J,I)
DO 307 I=1,MM
307 C(I)=QC(I)
GO TO 100
106 CONTINUE
END

```

SENTRY REGRES

6	46
2.00	1.10
2.20	1.10
2.40	1.10
2.60	1.10
2.80	1.10
3.00	1.10
2.80	1.20
2.60	1.20
2.40	1.20

2.6	1.200
2.80	1.200
3.00	1.200
2.60	1.400
2.20	1.400
2.40	1.400
2.60	1.400
2.80	1.400
3.00	1.400
2.60	1.600
2.20	1.600
2.40	1.600
2.60	1.600
2.80	1.600
3.00	1.600
2.00	1.800
2.20	1.800
2.40	1.800
2.60	1.800
2.80	1.800
3.00	1.800
2.00	2.000
2.20	2.000
2.40	2.000
2.60	2.000
2.80	2.000
3.00	2.000

(SAMPLE OUTPUT)

PROBLEM MULTIPLE REGRESSION BY LINEAR PROGRAMING.

OBJECTIVE VALUE = 0.7500000000
INDEP. VARIABLE 36 0.1000000000

OPTIMAL VALUE = 0.1000000000
INDEP. VARIABLE 36 0.1000000000
INDEP. VARIABLE 67 0.1000000000

5 5 5 5 5

OPTIMAL VALUE = 0.8000000000
INDEP. VARIABLE 36 0.8000000000
INDEP. VARIABLE 47 0.8000000000
INDEP. VARIABLE 1 0.0000000000

5 5 5 5 5

OPTIMAL VALUE = 0.1000000000

INDEP. VECTOR	36	0.23000000E-00
INDEP. VECTOR	42	0.23000000E-00
INDEP. VECTOR	7	0.23000000E-00
INDEP. VECTOR	67	0.23000000E-00

\$ \$ \$ \$ \$

OPTIMAL VALUE = 0.23000000E-00

INDEP. VECTOR	36	0.23000000E-00
INDEP. VECTOR	42	0.23000000E-00
INDEP. VECTOR	7	0.23000000E-00
INDEP. VECTOR	67	0.23000000E-00
INDEP. VECTOR	68	0.

THE FORM TO BE USED IS: 0. 5

\$ \$ \$ \$ \$

OPTIMAL VALUE = 0.23176474E-00

INDEP. VECTOR	32	0.23620583E-00
INDEP. VECTOR	42	0.23523477E-00
INDEP. VECTOR	7	0.26470589E-00
INDEP. VECTOR	67	0.26470589E-00
INDEP. VECTOR	24	0.23000000E-00

\$ \$ \$ \$ \$

OPTIMAL VALUE = 0.26624777E-00

INDEP. VECTOR	38	0.23783437E-00
INDEP. VECTOR	42	0.23474001E-00
INDEP. VECTOR	19	0.10697014E-00
INDEP. VECTOR	68	0.31500000E-00
INDEP. VECTOR	38	0.40000000E-00
INDEP. VECTOR	72	0.12400000E-00

\$ \$ \$ \$ \$

END OF PART FOUR (END OF 15).

PROBLEM PART II FOR MULTIPLE REGRESSION ANALYSIS.

- FINAL SOLUTIONS.
- 1. 32756284E-07
 - 2. 91300000E+00
 - 3. 70000000E+00
 - 4. 10000000E+00
 - 5. 92478235E-06
 - 6. 20000000E+00

λ	T	$F(\lambda, T)$	ΔL	Δd
2.1000	1.0000	4.4100	4.4000	1.0000
2.2000	1.0000	4.4100	4.4000	1.0000
2.4000	1.0000	4.4100	4.4000	1.0000
2.6000	1.0000	4.4100	4.4000	1.0000
2.8000	1.0000	4.4100	4.4000	1.0000
2.2000	1.2000	4.4100	4.4000	1.0000
2.4000	1.2000	4.4100	4.4000	1.0000
2.6000	1.2000	4.4100	4.4000	1.0000
2.8000	1.2000	4.4100	4.4000	1.0000
2.1000	1.4000	4.4100	4.4000	1.0000
2.2000	1.4000	4.4100	4.4000	1.0000
2.4000	1.4000	4.4100	4.4000	1.0000
2.6000	1.4000	4.4100	4.4000	1.0000
2.8000	1.4000	4.4100	4.4000	1.0000
2.1000	1.6000	4.4100	4.4000	1.0000
2.2000	1.6000	4.4100	4.4000	1.0000
2.4000	1.6000	4.4100	4.4000	1.0000
2.6000	1.6000	4.4100	4.4000	1.0000
2.8000	1.6000	4.4100	4.4000	1.0000
2.1000	1.8000	4.4100	4.4000	1.0000
2.2000	1.8000	4.4100	4.4000	1.0000
2.4000	1.8000	4.4100	4.4000	1.0000
2.6000	1.8000	4.4100	4.4000	1.0000
2.8000	1.8000	4.4100	4.4000	1.0000
2.1000	2.0000	4.4100	4.4000	1.0000
2.2000	2.0000	4.4100	4.4000	1.0000
2.4000	2.0000	4.4100	4.4000	1.0000
2.6000	2.0000	4.4100	4.4000	1.0000
2.8000	2.0000	4.4100	4.4000	1.0000

B29832